Supporting information

For

Impact of di- and poly-radical character on the relative energy of the doubly excited and L_a states of linear acenes and cyclacenes

Table S1: Energies of frontier molecular orbitals and H/L gap of **[n]-acenes** calculated at CS geometry (B3LYP/6-31G*). Orbital symmetries are indicated in parenthesis.

Molecule	CS geometry								
	L+3 (eV)	L+2 (eV)	L+1 (eV)	L (eV)	H (eV)	H-1 (eV)	H-2 (eV)	H-3 (eV)	ΔE (H/L) (eV)
[2]-acene	-	0.98 (B3U)	-0.15 (B2G)	-0.96 (B1G)	-5.79 (AU)	-6.54 (B3U)	-7.65 (B2G)	-	4.83
[4]-acene	-	-0.38 (B2G)	0.42 (B3U)	-2.08 (B1G)	-4.85 (AU)	-6.33 (B2G)	-6.41 (B3U)	-	2.78
[6]-acene	-	-0.48 (B2G)	-1.35 (B3U)	-2.61 (B1G)	-4.41 (AU)	-5.54 (B2G)	-6.36 (B3U)	-	1.80
[7]-acene	-0.51 (AU)	-0.60 (B3U)	-1.67 (B1G)	-2.78 (B3U)	-4.27 (B2G)	-5.27 (AU)	-6.21 (B2G)	-6.35 (B1G)	1.49
[8]-acene	-0.54 (B2G)	-0.94 (B1G)	-1.93 (B3U)	-2.91 (B1G)	-4.16 (AU)	-5.05 (B2G)	-5.92 (AU)	-6.34 (B3U)	1.25
[9]-acene	-0.56 (AU)	-1.23 (B3U)	-2.14 (B1G)	-3.01 (B3U)	-4.08 (B2G)	-4.87 (AU)	-5.67 (B2G)	-6.34 (B1G)	1.07

The inclusion of H-3, H-2, L+2 and L+3 orbitals is due to a different dependence of orbital energies on molecular size, already noticed by Marian and Gilka [1] and Bettinger *et al.*[2]. Considering naphthalene as our reference, its H-1 orbital becomes H-2 for tetracene and hexacene and H-3 for heptacene, octacene and nonacene; while its L+1 orbital will be L+2 orbital for tetracene and hexacene and L+3 for longer acenes. L and H orbitals are practically invariant.

Table S2: Energies of frontier molecular orbitals and H/L gap of **[n]-acenes** calculated at BS geometry (UB3LYP/6-31G*).

Molecule	BS geometry				
	L+1(eV)	L(eV)	H(eV)	H-1(eV)	ΔE (H/L) (eV)
[6]-acene	-1.34	-2.56	-4.46	-5.54	1.89
[7]-acene	-1.66	-2.60	-4.45	-5.27	1.86
[8]-acene	-1.91	-2.62	-4.46	-5.07	1.83
[9]-acene	-2.10	-2.64	-4.46	-4.91	1.82

Table S3: Frontier molecular orbital energies and H/L gap of (top) **even** and (bottom) **odd [n]-CCs** calculated at CS geometry (B3LYP/6-31G*). Where possible, orbital symmetries are indicated in parenthesis.

EVEN CC	CS geometry						
Molecule	**L+1(2)**	**L+1(1)**	**L**	**H**	**H-1(1)**	**H-1(2)**	**ΔE (H/L)**
[6]-CC	-	-1.71 (A1G)	-2.57 (B1G)	-3.81 (B2U)	-5.51 (E2U)	-5.51 (E2U)	1.24
[8]-CC	-1.71 (E3G)	-1.71 (E3G)	-2.79 (B1U)	-3.89 (B2G)	-4.96 (E3U)	-4.96 (E3U)	1.11
[10]-CC	-2.19 (E4G)	-2.19 (E4G)	-2.93 (B2G)	-3.93 (B1U)	-4.61 (E4U)	-4.61 (E4U)	1.00
[12]-CC	-2.54	-2.54	-3.03	-3.94	-4.37	-4.37	0.91

ODD CC	CS geometry								
Molecule	**L+1(1)**	**L+1(2)**	**L(1)**	**L(2)**	**H(1)**	**H(2)**	**H-1(1)**	**H-1(2)**	**ΔE (H/L)**
[7]-CC	-	-1.01 (A1')	-2.41 (E3')	-2.41 (E3')	-4.06 (E3")	-4.06 (E3")	-6.48 (E2")	-6.48 (E2")	1.65
[9]-CC	-0.94	-0.94	-2.79	-2.79	-3.92	-3.92	-5.83	-5.83	1.13
[11]-CC	-1.44	-1.44	-3.02	-3.02	-3.84	-3.84	-5.37	-5.37	0.82

Table S4: Frontier molecular orbital energies and H/L gap of (top) **even** and (bottom) **odd [n]-CCs** calculated at BS geometry (UB3LYP/6-31G*).

EVEN	BS geometry						
Molecule	**L+1(2)**	**L+1(1)**	**L**	**H**	**H-1(1)**	**H-1(2)**	**ΔE (H/L)**
[6]-CC	-	-1.68	-2.02	-4.29	-5.57	-5.57	2.27
[8]-CC	-1.58	-1.58	-2.30	-4.34	-5.06	-5.06	2.04
[10]-CC	-2.00	-2.00	-2.41	-4.41	-4.77	-4.77	2.00
[12]-CC	-2.26	-2.26	-2.45	-4.48	-4.61	-4.61	2.04

ODD	BS geometry								
Molecule	**L+1(1)**	**L+1(2)**	**L(1)**	**L(2)**	**H(1)**	**H(2)**	**H-1(1)**	**H-1(2)**	**ΔE (H/L)**
[7]-CC	-	-1.04	-2.07	-2.07	-4.40	-4.40	-6.43	-6.43	2.33
[9]-CC	-0.95	-0.95	-2.29	-2.29	-4.42	-4.42	-5.80	-5.80	2.13
[11]-CC	-1.43	-1.43	-2.42	-2.42	-4.44	-4.44	-5.37	-5.37	2.02

Table S5: Energies of (top) **[n]-acenes** and **[n]-CCs** at the optimized CS and BS geometries. CS wavefunctions computed with B3LYP, while BS wavefunctions are determined with UB3LYP functional. 6-31G* basis set is used. The percentage (%) is calculated as the ratio between ΔE(CS-BS) at CS geometry and that at BS geometry.

Molecule	CS geometry				BS geometry			
	E (CS) (a.u.)	E(BS) (a.u)	S**2 BS wavefunction	ΔE (CS-BS) (kcal/mol)	E(BS) (a.u)	S**2 BS wavefunction	ΔE (CS-BS) (kcal/mol)	%
[6]-acene	-1000.43348912	-1000.43360947	0.17	0.08	-1000.43368190	0.26	0.12	67
[7]-acene	-1154.06672393	-1154.06858321	0.61	1.17	-1154.06942602	0.80	1.70	69
[8]-acene	-1307.69978771	-1307.70456197	0.91	3.00	-1307.70624199	1.08	4.05	74
[9]-acene	-1461.33275688	-1461.34094364	1.13	5.14	-1461.34323692	1.26	6.58	78

Molecule	CS geometry				BS geometry			
	E (CS) (a.u.)	E(BS) (a.u)	S**2 BS wavefunction	ΔE (CS-BS) (kcal/mol)	E(BS) (a.u)	S**2 BS wavefunction	ΔE (CS-BS) (kcal/mol)	%
[6]-CC	-921.45884275	-921.47142897	1.16	7.90	-921.47164651	1.18	8.03	98
[7]-CC	-1075.13157369	-1075.14232577	1.59	6.75	-1075.14354825	1.72	7.51	90
[8]-CC	-1228.82283487	-1228.83447070	1.29	7.30	-1228.83463126	1.31	7.40	99
[9]-CC	-1382.46158009	-1382.48647919	2.17	15.62	-1382.48799130	2.24	16.57	94
[10]-CC	-1536.14403499	-1536.15802429	1.62	8.78	-1536.15826501	1.65	8.93	98
[11]-CC	-1689.76858012	-1689.80617543	2.48	23.59	-1689.80761244	2.52	24.49	96
[12]-CC	-1843.44463744	-1843.46370024	2.12	11.96	-1843.46413070	2.17	12.23	98

Table S6: Di- and poly-radical characters of **[n]-acenes** in terms of y_0, y_1 and N_{FOD}. y_0 and y_1 indexes are calculated at PUHF and PUB3LYP levels. N_{FOD} values are calculated at TPSS/def2-TZVP level with T_{el} set at 5000K. Both CS-B3LYP and BS-UB3LYP geometries are considered here.

Molecule ↓	$y_0^{(PUHF)}$		$y_0^{(PUB3LYP)}$		$y_1^{(PUHF)}$		$y_1^{(PUB3LYP)}$		N_{FOD}	
Geometry →	CS-B3LYP	BS-UB3LYP	CS-B3LYP	BS-UB3LYP	CS-B3LYP	BS-UB3LYP	CS-B3LYP	BS-UB3LYP	CS-B3LYP	BS-UB3LYP
[6]-acene	0.54	0.56	0	0.01	0.12	0.12	0	0	1.23	1.26
[7]-acene	0.64	0.70	0.06	0.13	0.18	0.18	0	0.001	1.60	1.71
[8]-acene	0.73	0.79	0.17	0.33	0.25	0.25	0.001	0.002	1.98	2.13
[9]-acene	0.79	0.86	0.33	0.54	0.32	0.33	0.004	0.005	2.35	2.52

Table S7: Di- and poly-radical characters of (top) even and (bottom) odd **[n]-CCs** in terms of y_0, y_1 and N_{FOD}. y_0 and y_1 indexes are calculated at PUHF and PUB3LYP levels. N_{FOD} values are calculated at TPSS/def2-TZVP level with T_{el} set at 5000K. Both CS-B3LYP and BS-UB3LYP geometries are considered here.

Molecule ↓	$y_0^{(PUHF)}$		$y_0^{(PUB3LYP)}$		$y_1^{(PUHF)}$		$y_1^{(PUB3LYP)}$		N_{FOD}	
Geometry →	CS-B3LYP	BS-UB3LYP	CS-B3LYP	BS-UB3LYP	CS-B3LYP	BS-UB3LYP	CS-B3LYP	BS-UB3LYP	CS-B3LYP	BS-UB3LYP
[6]-CC	0.84	0.85	0.37	0.39	0.16	0.16	0.001	0.001	1.77	1.79
[8]-CC	0.85	0.85	0.37	0.38	0.26	0.26	0.003	0.003	1.86	1.88
[10]-CC	0.85	0.86	0.40	0.41	0.39	0.40	0.012	0.013	2.43	2.46
[12]-CC	0.85	0.86	0.44	0.44	0.52	0.53	0.043	0.048	3.16	3.2
Molecule ↓	$y_0^{(PUHF)}$		$y_0^{(PUB3LYP)}$		$y_1^{(PUHF)}$		$y_1^{(PUB3LYP)}$		N_{FOD}	
Geometry →	CS-B3LYP	BS-UB3LYP	CS-B3LYP	BS-UB3LYP	CS-B3LYP	BS-UB3LYP	CS-B3LYP	BS-UB3LYP	CS-B3LYP	BS-UB3LYP
[7]-CC	0.67	0.69	0.14	0.18	0.67	0.69	0.138	0.176	2.53	2.66
[9]-CC	0.81	0.83	0.42	0.48	0.81	0.83	0.424	0.479	3.47	3.59
[11]-CC	0.90	0.91	0.72	0.77	0.90	0.91	0.716	0.767	4.27	4.38

Table S8: Expressions of the BS frontier molecular orbitals in terms of linear combination of CS frontier molecular orbitals.

$$H_\alpha = \varphi_{HOMO}^\alpha = \cos\theta \, H_{CS} + \sin\theta \, L_{CS}$$

$$H_\beta = \varphi_{HOMO}^\beta = \cos\theta \, H_{CS} - \sin\theta \, L_{CS}$$

$$L_\alpha = \varphi_{LUMO}^\alpha = \sin\theta \, H_{CS} - \cos\theta \, L_{CS}$$

$$L_\beta = \varphi_{LUMO}^\beta = \sin\theta \, H_{CS} + \cos\theta \, L_{CS}$$

Table S9: Excitation energies of the L_a state, dominated by the H→L excitation, for **[n]-acenes**, calculated at different levels of theory introduced in this work. Comparison with calculated data in literature and experimental results where possible.

La state	**This work**										
Molecule	DFT/MRCI R2018 [a]	DFT/MRCI Original [a]	TDB3LYP[a]	TDUB3LYP[a]	SF-TDB3LYP[a]	NEVPT2	TDPBE0-DH[b]	TDPBE-QIDH[b]	pp-RPA[c]	MCCEPA[d]	**Exp.**
[2]-acene	4.67	4.73	4.46	/	/	/	4.85	4.94	4.97	/	4.66[e]
[3]-acene	3.49	3.55	/	/	/	/	3.71	3.79	3.65	3.68	3.60[e]
[4]-acene	2.69	2.77	2.49	/	/	/	2.94	3.01	2.82	3.10	2.88[e]
[5]-acene	2.15	2.24	/	/	/	/	2.39	2.46	2.26	2.67	2.21[f]
[6]-acene	1.77	1.88	1.54	1.56	1.29	/	2.00	2.07	1.86	2.41	1.79[g]
[7]-acene	1.50	1.63	1.24	1.38	2.95	1.62[a]	/	/	1.58	2.27	1.65[d]
[8]-acene	1.32	1.47	1.00	1.30	0.73	1.39[a]	/	/	1.36	/	1.54[h]
[9]-acene	1.20	1.37	0.81	1.27	0.58	1.33[a]	/	/	1.20	/	1.43[h]

[a.] DFT/MRCI calculations carried out with def2-SVP basis set, while TDDFT-based calculations carried out with 6-31G* basis set; NEVPT2 calculations carried out with the strongly contracted variant. The (12,12) space was considered for **[7]-acene** and **[8]-acene**; for **[9]-acene**, the (14,14) space was used.

[b.] from ref. [3]. TDPBE0-DH calculations were carried out with def2-TZVP basis set, while TDPBE-QIDH used def2-QZVP basis set;

[c.] from ref. [4] considering the R geometry;

[d.] from ref. [5]; experimental result from UV-Vis absorption spectrum;

[e.] from ref. [6], derived from experimental 0-0 transition energy in solution;

[f.] from ref. [7], absorption in solid inert gas matrices at 10K;

[g.] from ref. [8], vertical S0→S1 energy;

[h.] from ref. [9], UV/Vis absorption spectra in solid Ar at 30K.

Table S10: Excitation energies of the DE state, dominated by the H,H→L,L excitation, for **[n]-acenes**, calculated at different levels of theory introduced in this work. Comparison with calculated data in literature and experimental results where possible. Energies of the $2A_g$ state of naphthalene calculated at DFT/MRCI level are shown in parenthesis.

DE (2AG) state	This work							
Molecule	DFT/MRCI R2018 [a]	DFT/MRCI Original [a]	TDUB3LYP[a]	SF-TDB3LYP[a]	NEVPT2	pp-RPA[b]	MCCEPA[c]	**Exp.**
[2]-acene	6.56 (5.96)	5.46 (5.80)	/	/	/	6.43	/	5.46[d]
[3]-acene	4.99	4.62	/	/	/	4.87	4.76	4.96[e]
[4]-acene	3.84	**3.43**	/	/	/	3.65	3.83	/
[5]-acene	2.93	**2.55**	/	/	/	2.74	2.92	/
[6]-acene	2.24	1.91	0.55	2.14	/	2.05	2.62	/
[7]-acene	1.73	1.45	0.95	1.46	1.82 [a]	1.54	2.10	1.57[c]
[8]-acene	1.34	1.13	1.09	1.02	1.44 [a]	1.14	/	/
[9]-acene	1.06	0.93	1.16	0.73	1.18 [a]	0.84	/	/

[a] DFT/MRCI calculations carried out with def2-SVP basis set, while TDUDFT and SF calculations carried out with 6-31G* basis set; NEVPT2 calculations carried out with the strongly contracted variant. The (12,12) space was considered for **[7]-acene** and **[8]-acene**; for **[9]-acene**, the (14,14) space was used.

[b] from ref. [4] considering the R geometry;

[c] from ref. [5]; experimental result from UV-Vis absorption spectrum;

[d] from ref. [10], two-photon absorption in cyclohexane;

[e] from ref. [11], two-photon absorption in cyclohexane.

Table S11: Excitation energies of the L_a state, dominated by the H→L excitation, and of the DE state, dominated by H,H →L,L excitation, for even **[n]-CCs**, calculated at different levels of theory introduced in this work.
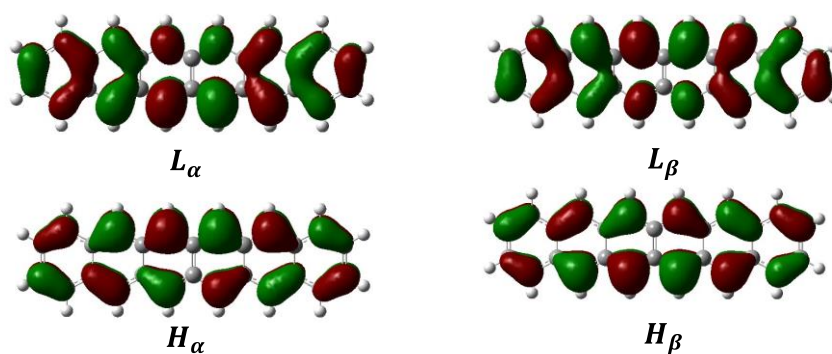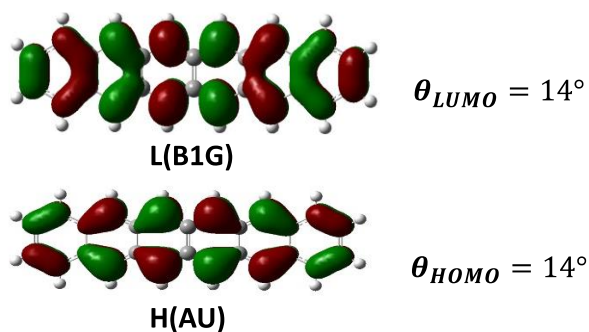
	La state					
Molecule	DFT/MRCI R2018 [a]	DFT/MRCI Original [a]	TDB3LYP/6-31G*	TDUB3LYP/6-31G*	SF-TDB3LYP/6-31G*	NEVPT2
[6]-CC	1.47	1.73	0.97	1.64	0.93	0.85 [b]
[8]-CC	1.33	1.54	0.82	1.47	0.79	0.85 [b]
[10]-CC	1.26	1.44	0.70	1.46	0.71	/
[12]-CC	1.22	1.39	0.60	1.51	0.65	/

	DE state				
Molecule	DFT/MRCI R2018	DFT/MRCI Original	TD-UB3LYP/6-31G*	SF-TD-B3LYP/6-31G*	NEVPT2
[6]-CC	1.72	1.49	1.49	1.25	1.18 [b]
[8]-CC	1.47	1.24	1.35	1.11	1.02 [b]
[10]-CC	1.24	1.03	1.40	1.02	0.85 [b]
[12]-CC	1.04	0.88	1.51	0.94	0.68 [b]

[a] DFT/MRCI calculations carried out with def2-SVP basis set.

[b] NEVPT2 calculations carried out with the strongly contracted variant. The (8,8) space was considered for **[6]-CC** and **[8]-CC**; for **[10]-CC** and **[12]-CC**, the (12,12) space was used.

[6]-acene

L(B1G)

$\theta_{LUMO} = 14°$

H(AU)

$\theta_{HOMO} = 14°$

L_α

L_β

H_α

H_β

[7]-acene

L(B3U)

$\theta_{LUMO} = 27°$

H(B2G)

$\theta_{HOMO} = 28°$

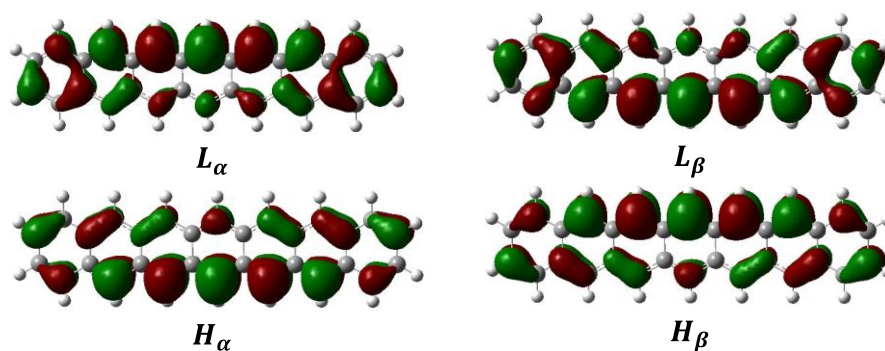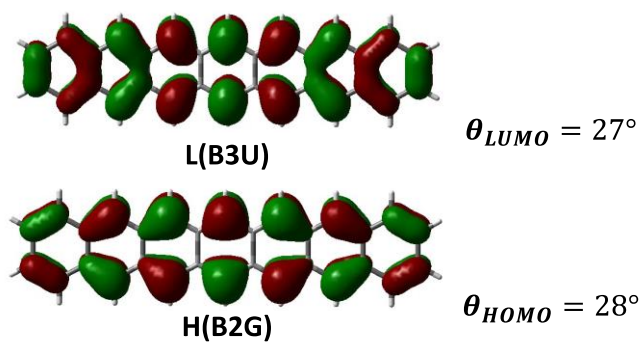L_α

L_β

H_α

H_β

Figure S1. Frontier molecular orbitals of **[n]-acenes**. (Top) Closed-shell (CS) orbitals computed at B3LYP; (bottom) Broken-symmetry (BS) orbitals obtained at UB3LYP level. 6-31G* basis set was used. Values of the rotation angle θ are also reported alongside the CS orbitals. Orbital symmetries are indicated in parenthesis.

[8]-acene

$\theta_{LUMO} = 33°$

L(B1G)

$\theta_{HOMO} = 35°$

H(AU)

L_α

L_β

H_α

H_β

[9]-acene

$\theta_{LUMO} = 38°$

L(B3U)

$\theta_{HOMO} = 39°$

H(B2G)

L_α

L_β

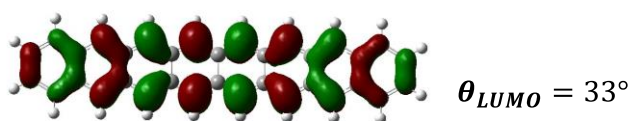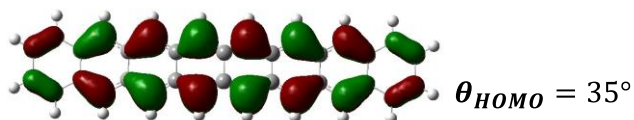H_α

H_β
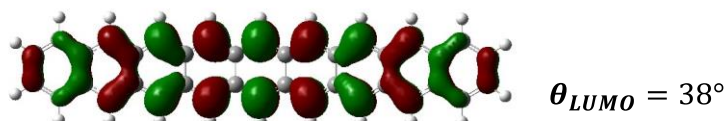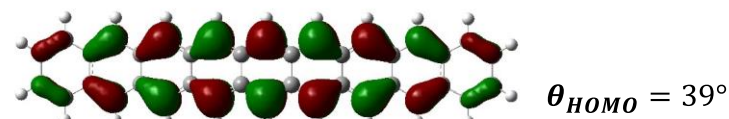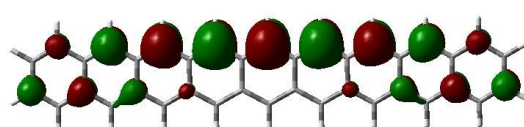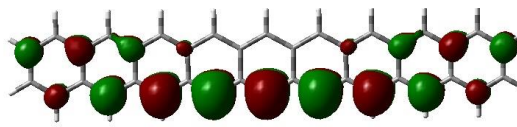
Figure S1_continued. Frontier molecular orbitals of **[n]-acenes**. (Top) Closed-shell (CS) orbitals computed at B3LYP; (bottom) Broken-symmetry (BS) orbitals obtained at UB3LYP level. 6-31G* basis set was used. Values of the rotation angle θ are also reported alongside the CS orbitals. Orbital symmetries are indicated in parenthesis.
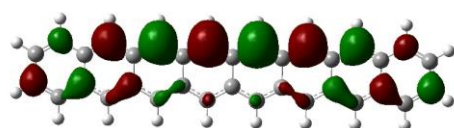
[6]-CC

$\theta_{LUMO} = 33°$

L (B1G)

$\theta_{HOMO} = 37°$

H (B2U)

L_α

L_β

H_α

H_β

[8]-CC

$\theta_{LUMO} = 32°$

L (B1U)

$\theta_{HOMO} = 37°$

H (B2G)

L_α

L_β

H_α

H_β

[10]-CC

$\theta_{LUMO} = 33°$

L (B2G)

$\theta_{HOMO} = 37°$

H (B1U)

L_α

L_β

H_α

H_β

[12]-CC

$\theta_{LUMO} = 33°$

L

$\theta_{HOMO} = 37°$

H

L_α

L_β

H_α

H_β
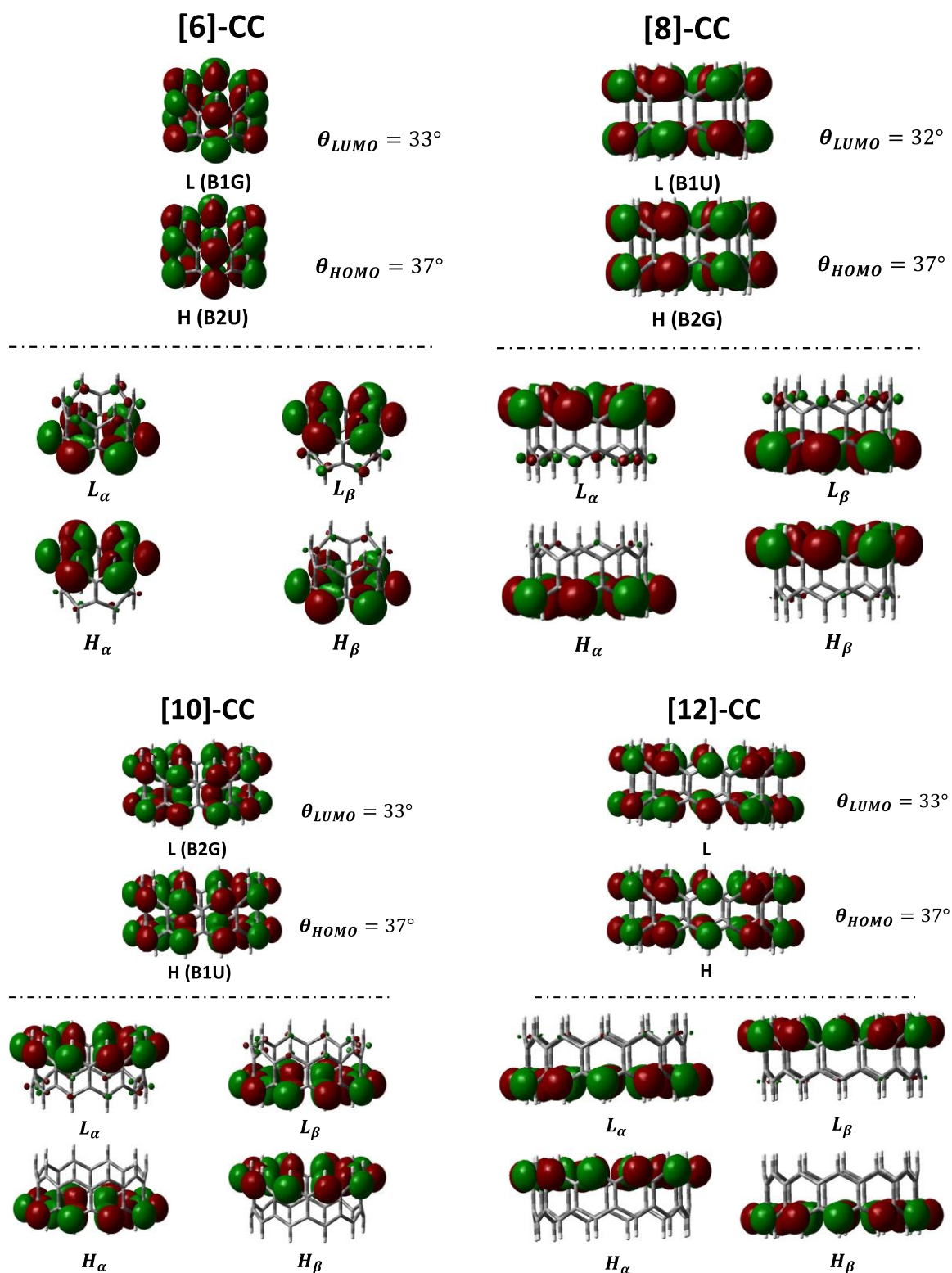
Figure S2. Frontier molecular orbitals of even **[n]-CCs**. (Top) Closed-shell (CS) orbitals computed at B3LYP; (bottom) Broken-symmetry (BS) orbitals obtained at UB3LYP level. 6-31G* basis set was used. Values of the rotation angle θ are also reported alongside the CS orbitals. Orbital symmetries are indicated in parenthesis.
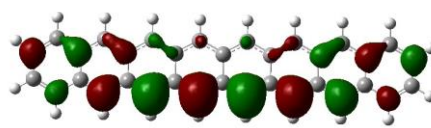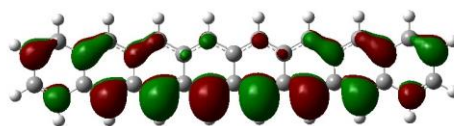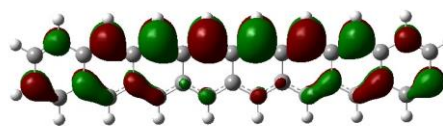
[7]-CC

L(2) (E3')   L(1) (E3')

H(2) (E3'')   H(1) (E3'')

$L(2)_\alpha$ $L(1)_\alpha$ $L(2)_\beta$ $L(1)_\beta$

$H(2)_\alpha$ $H(1)_\alpha$ $H(2)_\beta$ $H(1)_\beta$

[9]-CC

L(2)   L(1)

H(2)   H(1)

$L(2)_\alpha$ $L(1)_\alpha$ $L(2)_\beta$ $L(1)_\beta$

$H(2)_\alpha$ $H(1)_\alpha$ $H(2)_\beta$ $H(1)_\beta$
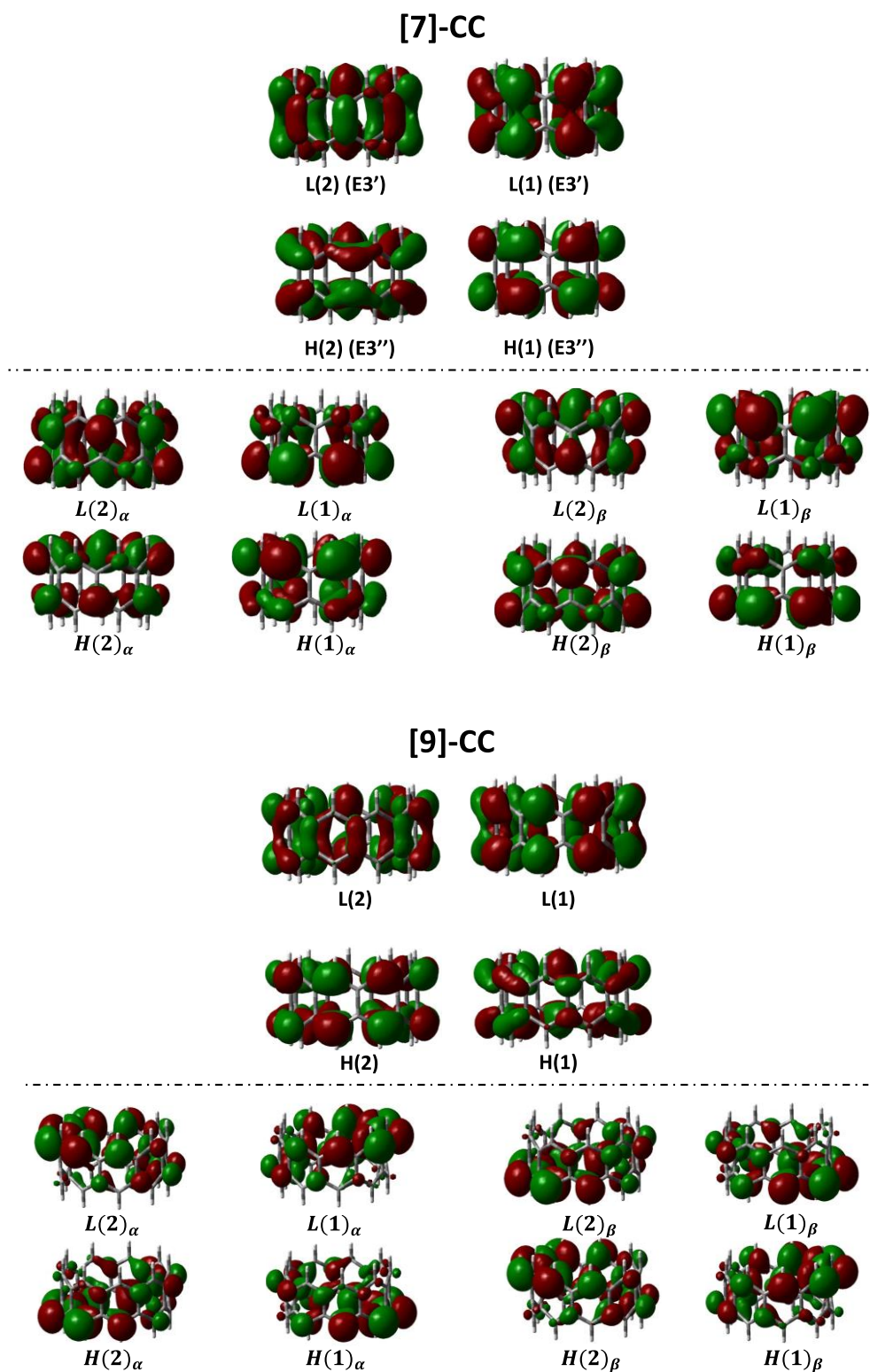
Figure S3. Frontier molecular orbitals of odd **[n]-CCs**. (Top) Closed-shell (CS) orbitals computed at B3LYP; (bottom) Broken-symmetry (BS) orbitals obtained at UB3LYP level. 6-31G* basis set was used. Orbital symmetries are indicated in parenthesis where possible.

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[11]-CC

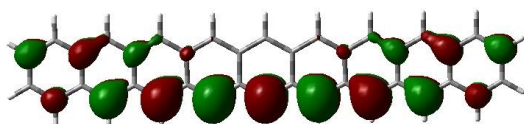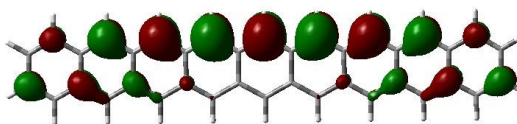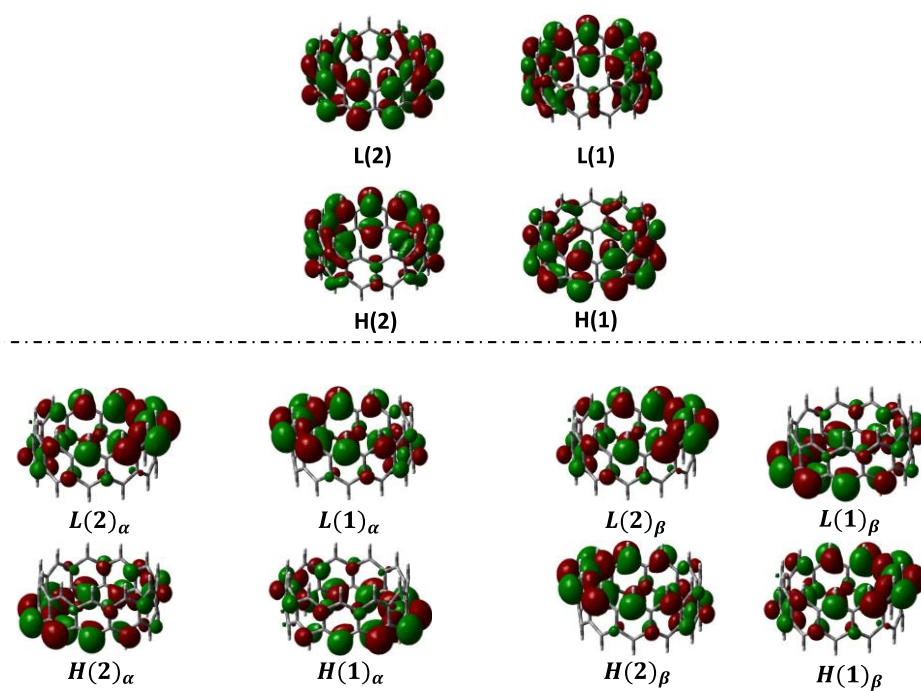**Figure S3_continued.** Frontier molecular orbitals of odd **[n]-CCs**. (Top) Closed-shell (CS) orbitals computed at B3LYP; (bottom) Broken-symmetry (BS) orbitals obtained at UB3LYP level. 6-31G* basis set was used. Orbital symmetries are indicated in parenthesis where possible.
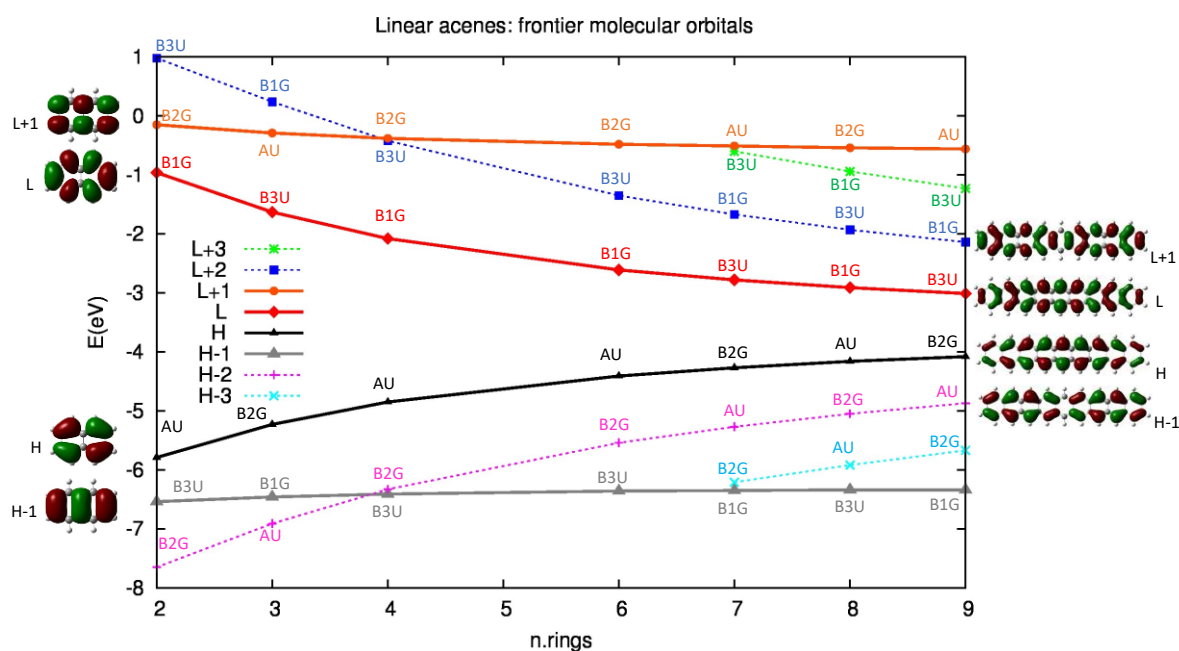
Figure S4. Ordering of frontier molecular orbitals (FMOs) of **[n]-acenes** calculated at B3LYP/6-31G* level. Symmetries are labeled above or under the line with the same color. Left: four FMOs of naphthalene (**[2]-acene**); right: four FMOs of nonacene (**[9]-acene**).

In Figure S4, orbitals with electronic distributions similar to that of naphthalene's four frontier molecular orbitals (FMOs) are represented by solid line. Note that the switch of FMOs' order of larger acenes is mainly due to the energy decreasing of other orbitals (*e.g.* H-1 and L+1 of longer acenes) as the molecular size increases. These orbitals become more and more relevant for the description of low-lying excited states of longer acenes and in particular, for the description of the DE state, as discussed in previous work[4].
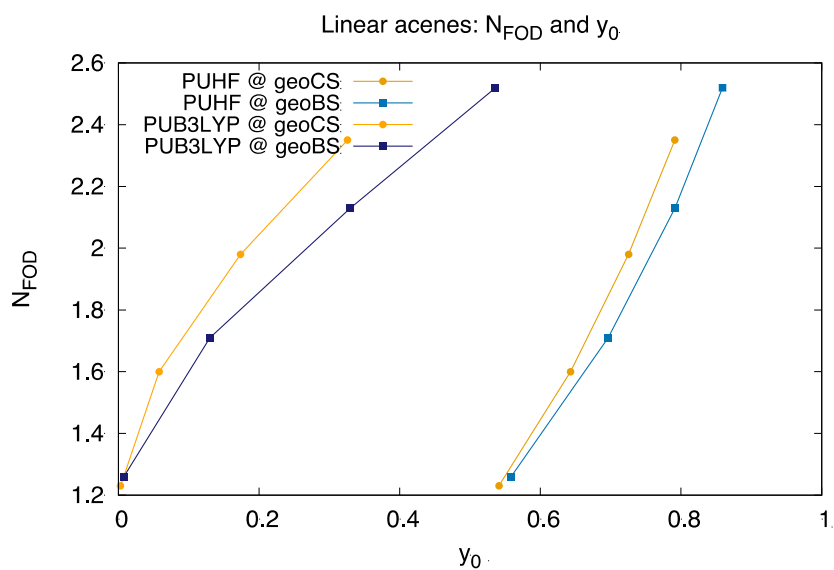
Figure S5. Relationship between N_{FOD} values and y_0 values for **[n]-acenes**. y_0 were calculated both at PUHF/6-31G* (gold and blue lines) and PUB3LYP/6-31G* (orange and midnight blue lines) levels. Two geometries were considered: CS-B3LYP (circles) and BS-UB3LYP (squares).
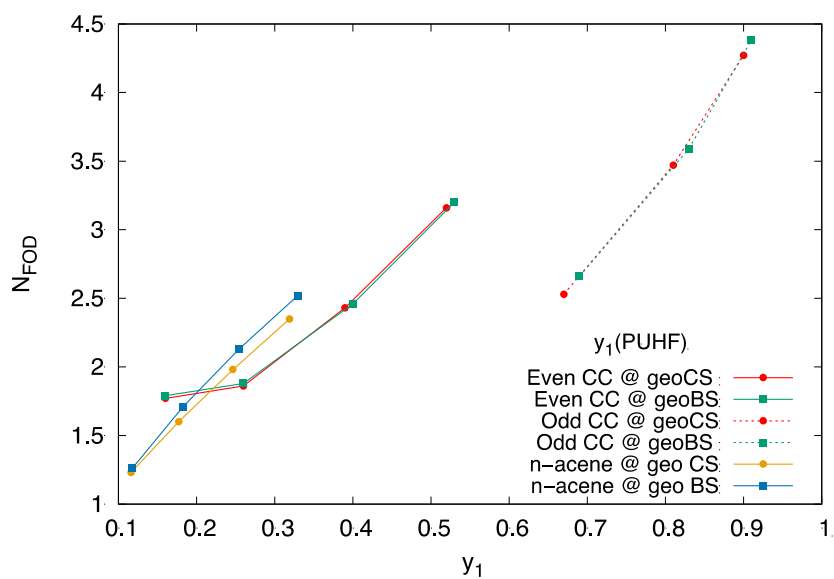
Figure S6. Relationship between N_{FOD} values and y_1^{PUHF} for even **[n]-CCs** (solid red and green lines), odd **[n]-CCs** (dashed red and green lines) and **[n]-acenes** (solid gold and blue lines). Two geometries were considered: CS-B3LYP (circles) and BS-UB3LYP (squares).
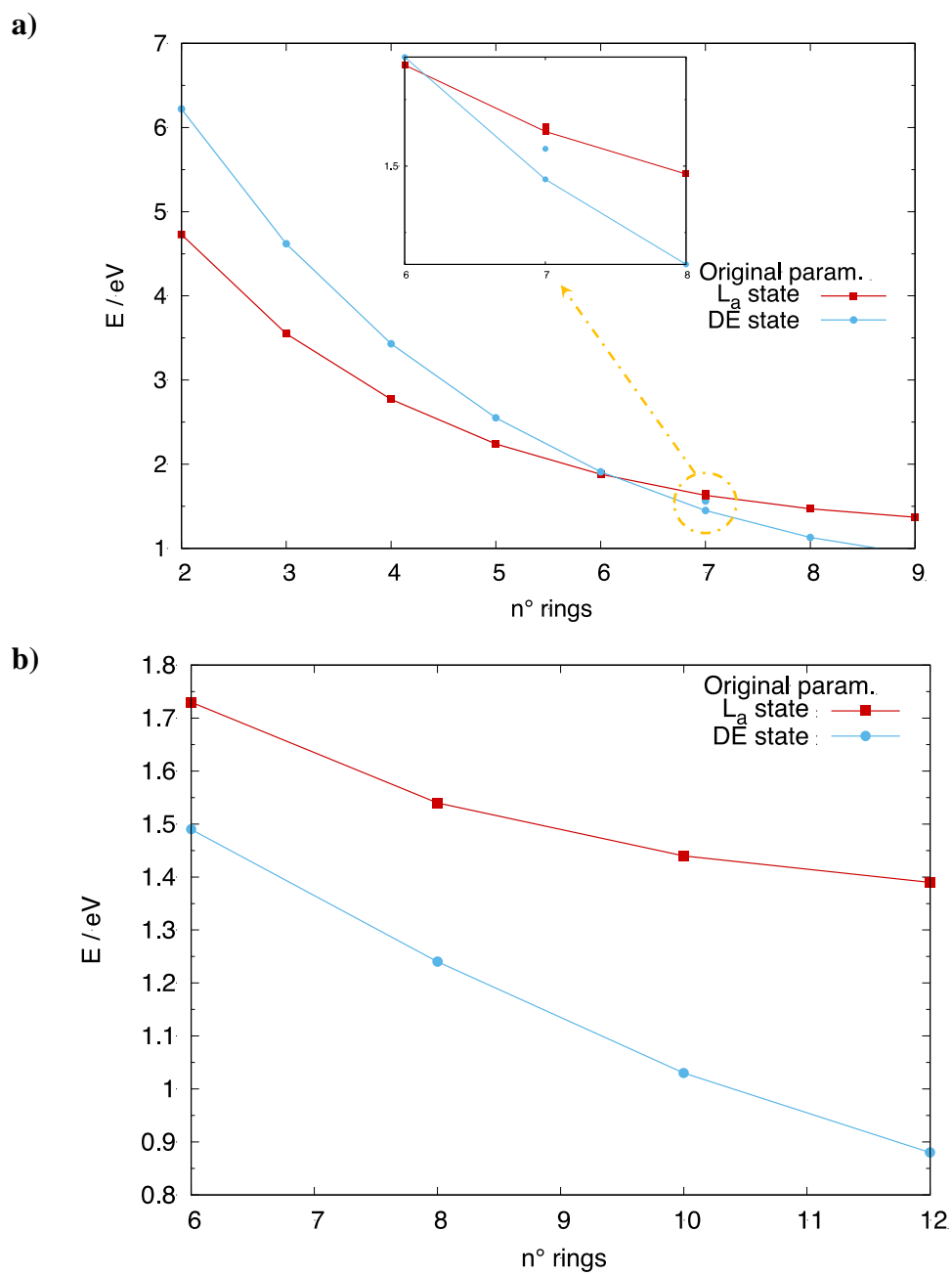
Figure S7. Crossing between the L_a and DE states predicted by DFT/MRCI calculations with the original parametrization: (**a**) **[n]-acenes**: The isolated cyan and red data points correspond to experimental data from ref. [5]; (**b**) **[n]-CCs**.

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Cartesian coordinates

[2]-acene: CS-B3LYP geometry

C	0.000000	0.000000	0.717142
C	0.000000	0.000000	-0.717142
C	0.000000	1.244511	-1.402567
C	0.000000	2.433524	-0.708529
C	0.000000	2.433524	0.708529
C	0.000000	1.244511	1.402567
H	0.000000	1.242065	-2.490240
H	0.000000	3.377852	-1.246300
H	0.000000	3.377852	1.246300
H	0.000000	1.242065	2.490240
C	0.000000	-1.244511	-1.402567
C	0.000000	-2.433524	-0.708529
H	0.000000	-3.377852	-1.246300
C	0.000000	-2.433524	0.708529
H	0.000000	-3.377852	1.246300
C	0.000000	-1.244511	1.402567
H	0.000000	-1.242065	-2.490240
H	0.000000	-1.242065	2.490240

[3]-acene: CS-B3LYP geometry

C	0.000000	3.660679	0.713146
C	0.000000	2.479530	1.407036
C	0.000000	1.223923	0.722624
C	0.000000	1.223923	-0.722624
C	0.000000	2.479530	-1.407036
C	0.000000	3.660679	-0.713146
C	0.000000	0.000000	1.403377
C	0.000000	0.000000	-1.403377
C	0.000000	-1.223923	-0.722624
C	0.000000	-1.223923	0.722624
C	0.000000	-2.479530	1.407036
H	0.000000	-2.476865	2.494579
C	0.000000	-3.660679	0.713146
C	0.000000	-3.660679	-0.713146
C	0.000000	-2.479530	-1.407036
H	0.000000	0.000000	2.491747
H	0.000000	4.607360	1.246657
H	0.000000	2.476865	2.494579
H	0.000000	2.476865	-2.494579
H	0.000000	4.607360	-1.246657
H	0.000000	0.000000	-2.491747

```
H    0.000000    -4.607360     1.246657
H    0.000000    -4.607360    -1.246657
H    0.000000    -2.476865    -2.494579
```

[4]-acene: CS-B3LYP geometry

```
C    0.000000     2.450756     0.726095
C    0.000000     2.450756    -0.726095
C    0.000000     3.711077    -1.409420
C    0.000000     4.888961    -0.715531
C    0.000000     4.888961     0.715531
C    0.000000     3.711077     1.409420
H    0.000000     3.708826    -2.496975
H    0.000000     5.836351    -1.247827
H    0.000000     5.836351     1.247827
H    0.000000     3.708826     2.496975
C    0.000000     1.235149    -1.406273
C    0.000000     0.000000    -0.726164
C    0.000000     0.000000     0.726164
C    0.000000     1.235149     1.406273
H    0.000000     1.234986    -2.494546
H    0.000000     1.234986     2.494546
C    0.000000    -1.235149     1.406273
C    0.000000    -2.450756     0.726095
C    0.000000    -2.450756    -0.726095
C    0.000000    -1.235149    -1.406273
H    0.000000    -1.234986     2.494546
H    0.000000    -1.234986    -2.494546
C    0.000000    -3.711077     1.409420
C    0.000000    -4.888961     0.715531
H    0.000000    -5.836351     1.247827
C    0.000000    -4.888961    -0.715531
H    0.000000    -5.836351    -1.247827
C    0.000000    -3.711077    -1.409420
H    0.000000    -3.708826     2.496975
H    0.000000    -3.708826    -2.496975
```

[5]-acene: CS-B3LYP geometry

```
C    0.000000     3.678641     0.727804
C    0.000000     3.678641    -0.727804
C    0.000000     4.941854    -1.410435
C    0.000000     6.117937    -0.716521
C    0.000000     6.117937     0.716521
```

C	0.000000	4.941854	1.410435
H	0.000000	4.939926	-2.497957
H	0.000000	7.065852	-1.247836
H	0.000000	7.065852	1.247836
H	0.000000	4.939926	2.497957
C	0.000000	2.467521	-1.407848
C	0.000000	1.226219	-0.728407
C	0.000000	1.226219	0.728407
C	0.000000	2.467521	1.407848
H	0.000000	2.466983	-2.496030
H	0.000000	2.466983	2.496030
C	0.000000	0.000000	1.408703
C	0.000000	-1.226219	0.728407
C	0.000000	-1.226219	-0.728407
C	0.000000	0.000000	-1.408703
H	0.000000	0.000000	2.496622
H	0.000000	0.000000	-2.496622
C	0.000000	-2.467521	1.407848
C	0.000000	-3.678641	0.727804
C	0.000000	-3.678641	-0.727804
C	0.000000	-2.467521	-1.407848
H	0.000000	-2.466983	2.496030
H	0.000000	-2.466983	-2.496030
C	0.000000	-4.941854	1.410435
C	0.000000	-6.117937	0.716521
H	0.000000	-7.065852	1.247836
C	0.000000	-6.117937	-0.716521
H	0.000000	-7.065852	-1.247836
C	0.000000	-4.941854	-1.410435
H	0.000000	-4.939926	2.497957
H	0.000000	-4.939926	-2.497957

[6]-acene: CS-B3LYP geometry

C	0.000000	4.907374	0.728592
C	0.000000	4.907374	-0.728592
C	0.000000	6.171739	-1.411088
C	0.000000	7.346953	-0.717126
C	0.000000	7.346953	0.717126
C	0.000000	6.171739	1.411088
H	0.000000	6.169623	-2.498584
H	0.000000	8.295243	-1.247691
H	0.000000	8.295243	1.247691
H	0.000000	6.169623	2.498584
C	0.000000	3.698528	-1.408803

```
C    0.000000    2.454423    -0.729833
C    0.000000    2.454423    0.729833
C    0.000000    3.698528    1.408803
H    0.000000    3.698509    -2.496949
H    0.000000    3.698509    2.496949
C    0.000000    1.232356    1.409788
C    0.000000    0.000000    0.730648
C    0.000000    0.000000    -0.730648
C    0.000000    1.232356    -1.409788
H    0.000000    1.232675    2.497822
H    0.000000    1.232675    -2.497822
C    0.000000    -1.232356    1.409788
C    0.000000    -2.454423    0.729833
C    0.000000    -2.454423    -0.729833
C    0.000000    -1.232356    -1.409788
H    0.000000    -1.232675    2.497822
H    0.000000    -1.232675    -2.497822
C    0.000000    -3.698528    1.408803
C    0.000000    -4.907374    0.728592
C    0.000000    -4.907374    -0.728592
C    0.000000    -3.698528    -1.408803
H    0.000000    -3.698509    2.496949
H    0.000000    -3.698509    -2.496949
C    0.000000    -6.171739    1.411088
C    0.000000    -7.346953    0.717126
H    0.000000    -8.295243    1.247691
C    0.000000    -7.346953    -0.717126
H    0.000000    -8.295243    -1.247691
C    0.000000    -6.171739    -1.411088
H    0.000000    -6.169623    2.498584
H    0.000000    -6.169623    -2.498584
```

[6]-acene: BS-UB3LYP geometry

```
C    0.000000    4.911463    0.727189
C    0.000000    4.911463    -0.727189
C    0.000000    6.172948    -1.409909
C    0.000000    7.350440    -0.715865
C    0.000000    7.350440    0.715865
C    0.000000    6.172948    1.409909
H    0.000000    6.170501    -2.497429
H    0.000000    8.298208    -1.247287
H    0.000000    8.298208    1.247287
H    0.000000    6.170501    2.497429
C    0.000000    3.698483    -1.407950
```

```
C    0.000000    2.457538    -0.729286
C    0.000000    2.457538     0.729286
C    0.000000    3.698483     1.407950
H    0.000000    3.698326    -2.496151
H    0.000000    3.698326     2.496151
C    0.000000    1.232111     1.409764
C    0.000000    0.000000     0.730405
C    0.000000    0.000000    -0.730405
C    0.000000    1.232111    -1.409764
H    0.000000    1.232148     2.497796
H    0.000000    1.232148    -2.497796
C    0.000000   -1.232111     1.409764
C    0.000000   -2.457538     0.729286
C    0.000000   -2.457538    -0.729286
C    0.000000   -1.232111    -1.409764
H    0.000000   -1.232148     2.497796
H    0.000000   -1.232148    -2.497796
C    0.000000   -3.698483     1.407950
C    0.000000   -4.911463     0.727189
C    0.000000   -4.911463    -0.727189
C    0.000000   -3.698483    -1.407950
H    0.000000   -3.698326     2.496151
H    0.000000   -3.698326    -2.496151
C    0.000000   -6.172948     1.409909
C    0.000000   -7.350440     0.715865
H    0.000000   -8.298208     1.247287
C    0.000000   -7.350440    -0.715865
H    0.000000   -8.298208    -1.247287
C    0.000000   -6.172948    -1.409909
H    0.000000   -6.170501     2.497429
H    0.000000   -6.170501    -2.497429
```

[7]-acene: CS-B3LYP geometry

```
C    0.000000    6.136520    0.729112
C    0.000000    6.136520   -0.729112
C    0.000000    7.401543   -1.411491
C    0.000000    8.576302   -0.717513
C    0.000000    8.576302    0.717513
C    0.000000    7.401543    1.411491
H    0.000000    7.399614   -2.498970
H    0.000000    9.524678   -1.247881
H    0.000000    9.524678    1.247881
H    0.000000    7.399614    2.498970
C    0.000000    4.928757   -1.409253
```

C	0.000000	3.683061	-0.730602
C	0.000000	3.683061	0.730602
C	0.000000	4.928757	1.409253
H	0.000000	4.928927	-2.497411
H	0.000000	4.928927	2.497411
C	0.000000	2.463332	1.410508
C	0.000000	1.227899	0.731585
C	0.000000	1.227899	-0.731585
C	0.000000	2.463332	-1.410508
H	0.000000	2.463595	2.498521
H	0.000000	2.463595	-2.498521
C	0.000000	0.000000	1.410845
C	0.000000	-1.227899	0.731585
C	0.000000	-1.227899	-0.731585
C	0.000000	0.000000	-1.410845
H	0.000000	0.000000	2.498834
H	0.000000	0.000000	-2.498834
C	0.000000	-2.463332	1.410508
C	0.000000	-3.683061	0.730602
C	0.000000	-3.683061	-0.730602
C	0.000000	-2.463332	-1.410508
H	0.000000	-2.463595	2.498521
H	0.000000	-2.463595	-2.498521
C	0.000000	-4.928757	1.409253
C	0.000000	-6.136520	0.729112
C	0.000000	-6.136520	-0.729112
C	0.000000	-4.928757	-1.409253
H	0.000000	-4.928927	2.497411
H	0.000000	-4.928927	-2.497411
C	0.000000	-7.401543	1.411491
C	0.000000	-8.576302	0.717513
H	0.000000	-9.524678	1.247881
C	0.000000	-8.576302	-0.717513
H	0.000000	-9.524678	-1.247881
C	0.000000	-7.401543	-1.411491
H	0.000000	-7.399614	-2.498970
H	0.000000	-7.399614	2.498970

[7]-acene: BS-UB3LYP geometry

C	0.000000	6.150238	0.724952
C	0.000000	6.150238	-0.724952
C	0.000000	7.407114	-1.408013
C	0.000000	8.588251	-0.713677
C	0.000000	8.588251	0.713677

C	0.000000	7.407114	1.408013
H	0.000000	7.404688	-2.495530
H	0.000000	9.535077	-1.246787
H	0.000000	9.535077	1.246787
H	0.000000	7.404688	2.495530
C	0.000000	4.930309	-1.406557
C	0.000000	3.695364	-0.728308
C	0.000000	3.695364	0.728308
C	0.000000	4.930309	1.406557
H	0.000000	4.930721	-2.494729
H	0.000000	4.930721	2.494729
C	0.000000	2.462903	1.409305
C	0.000000	1.232941	0.731128
C	0.000000	1.232941	-0.731128
C	0.000000	2.462903	-1.409305
H	0.000000	2.463500	2.497279
H	0.000000	2.463500	-2.497279
C	0.000000	0.000000	1.410355
C	0.000000	-1.232941	0.731128
C	0.000000	-1.232941	-0.731128
C	0.000000	0.000000	-1.410355
H	0.000000	0.000000	2.498278
H	0.000000	0.000000	-2.498278
C	0.000000	-2.462903	1.409305
C	0.000000	-3.695364	0.728308
C	0.000000	-3.695364	-0.728308
C	0.000000	-2.462903	-1.409305
H	0.000000	-2.463500	2.497279
H	0.000000	-2.463500	-2.497279
C	0.000000	-4.930309	1.406557
C	0.000000	-6.150238	0.724952
C	0.000000	-6.150238	-0.724952
C	0.000000	-4.930309	-1.406557
H	0.000000	-4.930721	2.494729
H	0.000000	-4.930721	-2.494729
C	0.000000	-7.407114	1.408013
C	0.000000	-8.588251	0.713677
H	0.000000	-9.535077	1.246787
C	0.000000	-8.588251	-0.713677
H	0.000000	-9.535077	-1.246787
C	0.000000	-7.407114	-1.408013
H	0.000000	-7.404688	-2.495530
H	0.000000	-7.404688	2.495530

[8]-acene: CS-B3LYP geometry

24

C	0.000000	7.366104	0.729405
C	0.000000	7.366104	-0.729405
C	0.000000	9.805838	-0.717701
C	0.000000	9.805838	0.717701
C	0.000000	8.631529	1.411638
H	0.000000	10.754274	-1.247984
H	0.000000	10.754274	1.247984
H	0.000000	8.629626	2.499130
C	0.000000	6.158802	-1.409500
C	0.000000	4.912204	-0.731024
C	0.000000	4.912204	0.731024
C	0.000000	6.158802	1.409500
H	0.000000	6.158970	-2.497649
H	0.000000	6.158970	2.497649
C	0.000000	3.693947	1.410862
C	0.000000	2.456747	0.732198
C	0.000000	2.456747	-0.732198
C	0.000000	3.693947	-1.410862
H	0.000000	3.694059	2.498865
H	0.000000	3.694059	-2.498865
C	0.000000	1.231221	1.411425
C	0.000000	0.000000	0.732577
C	0.000000	0.000000	-0.732577
C	0.000000	1.231221	-1.411425
H	0.000000	1.231120	2.499399
H	0.000000	1.231120	-2.499399
C	0.000000	-1.231221	1.411425
C	0.000000	-2.456747	0.732198
C	0.000000	-2.456747	-0.732198
C	0.000000	-1.231221	-1.411425
H	0.000000	-1.231120	2.499399
H	0.000000	-1.231120	-2.499399
C	0.000000	-3.693947	1.410862
C	0.000000	-4.912204	0.731024
C	0.000000	-4.912204	-0.731024
C	0.000000	-3.693947	-1.410862
H	0.000000	-3.694059	2.498865
H	0.000000	-3.694059	-2.498865
C	0.000000	-6.158802	1.409500
C	0.000000	-7.366104	0.729405
C	0.000000	-7.366104	-0.729405
C	0.000000	-6.158802	-1.409500
H	0.000000	-6.158970	-2.497649
H	0.000000	-6.158970	2.497649
C	0.000000	-8.631529	-1.411638
C	0.000000	-9.805838	-0.717701
H	0.000000	-10.754274	-1.247984

C	0.000000	-9.805838	0.717701
H	0.000000	-10.754274	1.247984
C	0.000000	-8.631529	1.411638
H	0.000000	-8.629626	-2.499130
H	0.000000	-8.629626	2.499130
C	0.000000	8.631529	-1.411638
H	0.000000	8.629626	-2.499130

[8]-acene: BS-UB3LYP geometry

C	0.000000	7.384600	0.724225
C	0.000000	7.384600	-0.724225
C	0.000000	9.822225	-0.713110
C	0.000000	9.822225	0.713110
C	0.000000	8.640213	1.407485
H	0.000000	10.768840	-1.246594
H	0.000000	10.768840	1.246594
H	0.000000	8.637682	2.495005
C	0.000000	6.162609	-1.405958
C	0.000000	4.930212	-0.727590
C	0.000000	4.930212	0.727590
C	0.000000	6.162609	1.405958
H	0.000000	6.162929	-2.494143
H	0.000000	6.162929	2.494143
C	0.000000	3.694197	1.408669
C	0.000000	2.467774	0.730752
C	0.000000	2.467774	-0.730752
C	0.000000	3.694197	-1.408669
H	0.000000	3.694762	2.496668
H	0.000000	3.694762	-2.496668
C	0.000000	1.230787	1.409989
C	0.000000	0.000000	0.731843
C	0.000000	0.000000	-0.731843
C	0.000000	1.230787	-1.409989
H	0.000000	1.230962	2.497928
H	0.000000	1.230962	-2.497928
C	0.000000	-1.230787	1.409989
C	0.000000	-2.467774	0.730752
C	0.000000	-2.467774	-0.730752
C	0.000000	-1.230787	-1.409989
H	0.000000	-1.230962	2.497928
H	0.000000	-1.230962	-2.497928
C	0.000000	-3.694197	1.408669
C	0.000000	-4.930212	0.727590
C	0.000000	-4.930212	-0.727590
C	0.000000	-3.694197	-1.408669

H	0.000000	-3.694762	2.496668
H	0.000000	-3.694762	-2.496668
C	0.000000	-6.162609	1.405958
C	0.000000	-7.384600	0.724225
C	0.000000	-7.384600	-0.724225
C	0.000000	-6.162609	-1.405958
H	0.000000	-6.162929	-2.494143
H	0.000000	-6.162929	2.494143
C	0.000000	-8.640213	-1.407485
C	0.000000	-9.822225	-0.713110
H	0.000000	-10.768840	-1.246594
C	0.000000	-9.822225	0.713110
H	0.000000	-10.768840	1.246594
C	0.000000	-8.640213	1.407485
H	0.000000	-8.637682	-2.495005
H	0.000000	-8.637682	2.495005
C	0.000000	8.640213	-1.407485
H	0.000000	8.637682	-2.495005

[9]-acene: CS-B3LYP geometry

C	0.000000	6.141286	0.731266
C	0.000000	6.141286	-0.731266
C	0.000000	8.595146	-0.729743
C	0.000000	8.595146	0.729743
C	0.000000	7.388434	1.409718
H	0.000000	7.388614	2.497875
C	0.000000	4.923646	-1.411168
C	0.000000	3.685499	-0.732579
C	0.000000	3.685499	0.732579
C	0.000000	4.923646	1.411168
H	0.000000	4.923911	-2.499149
H	0.000000	4.923911	2.499149
C	0.000000	2.461374	1.411808
C	0.000000	1.228570	0.733068
C	0.000000	1.228570	-0.733068
C	0.000000	2.461374	-1.411808
H	0.000000	2.461411	2.499762
H	0.000000	2.461411	-2.499762
C	0.000000	0.000000	1.412085
C	0.000000	-1.228570	0.733068
C	0.000000	-1.228570	-0.733068
C	0.000000	0.000000	-1.412085
H	0.000000	0.000000	2.500017
H	0.000000	0.000000	-2.500017
C	0.000000	-2.461374	1.411808

```
C    0.000000    -3.685499     0.732579
C    0.000000    -3.685499    -0.732579
C    0.000000    -2.461374    -1.411808
H    0.000000    -2.461411     2.499762
H    0.000000    -2.461411    -2.499762
C    0.000000    -4.923646     1.411168
C    0.000000    -6.141286     0.731266
C    0.000000    -6.141286    -0.731266
C    0.000000    -4.923646    -1.411168
H    0.000000    -4.923911     2.499149
H    0.000000    -4.923911    -2.499149
C    0.000000    -7.388434     1.409718
C    0.000000    -8.595146     0.729743
C    0.000000    -8.595146    -0.729743
C    0.000000    -7.388434    -1.409718
H    0.000000    -7.388614    -2.497875
H    0.000000    -7.388614     2.497875
C    0.000000    -9.860861    -1.411905
C    0.000000   -11.035072    -0.717839
H    0.000000   -11.983705    -1.247717
C    0.000000   -11.035072     0.717839
H    0.000000   -11.983705     1.247717
C    0.000000    -9.860861     1.411905
H    0.000000    -9.859005    -2.499383
H    0.000000    -9.859005     2.499383
C    0.000000     7.388434    -1.409718
H    0.000000     7.388614    -2.497875
C    0.000000     9.860861    -1.411905
C    0.000000    11.035072    -0.717839
H    0.000000    11.983705    -1.247717
C    0.000000    11.035072     0.717839
H    0.000000    11.983705     1.247717
C    0.000000     9.860861     1.411905
H    0.000000     9.859005     2.499383
H    0.000000     9.859005    -2.499383
```

[9]-acene: BS-UB3LYP geometry

```
C    0.000000     6.163081     0.727294
C    0.000000     6.163081    -0.727294
C    0.000000     8.617012    -0.724113
C    0.000000     8.617012     0.724113
C    0.000000     7.394864     1.405807
H    0.000000     7.395092     2.493997
C    0.000000     4.925998    -1.408333
```

C	0.000000	3.701540	-0.730328
C	0.000000	3.701540	0.730328
C	0.000000	4.925998	1.408333
H	0.000000	4.926420	-2.496352
H	0.000000	4.926420	2.496352
C	0.000000	2.461835	1.409527
C	0.000000	1.234448	0.731690
C	0.000000	1.234448	-0.731690
C	0.000000	2.461835	-1.409527
H	0.000000	2.461930	2.497499
H	0.000000	2.461930	-2.497499
C	0.000000	0.000000	1.409760
C	0.000000	-1.234448	0.731690
C	0.000000	-1.234448	-0.731690
C	0.000000	0.000000	-1.409760
H	0.000000	0.000000	2.497723
H	0.000000	0.000000	-2.497723
C	0.000000	-2.461835	1.409527
C	0.000000	-3.701540	0.730328
C	0.000000	-3.701540	-0.730328
C	0.000000	-2.461835	-1.409527
H	0.000000	-2.461930	2.497499
H	0.000000	-2.461930	-2.497499
C	0.000000	-4.925998	1.408333
C	0.000000	-6.163081	0.727294
C	0.000000	-6.163081	-0.727294
C	0.000000	-4.925998	-1.408333
H	0.000000	-4.926420	2.496352
H	0.000000	-4.926420	-2.496352
C	0.000000	-7.394864	1.405807
C	0.000000	-8.617012	0.724113
C	0.000000	-8.617012	-0.724113
C	0.000000	-7.394864	-1.405807
H	0.000000	-7.395092	-2.493997
H	0.000000	-7.395092	2.493997
C	0.000000	-9.872578	-1.407452
C	0.000000	-11.054548	-0.713100
H	0.000000	-12.001164	-1.246583
C	0.000000	-11.054548	0.713100
H	0.000000	-12.001164	1.246583
C	0.000000	-9.872578	1.407452
H	0.000000	-9.870003	-2.494972
H	0.000000	-9.870003	2.494972
C	0.000000	7.394864	-1.405807
H	0.000000	7.395092	-2.493997
C	0.000000	9.872578	-1.407452
C	0.000000	11.054548	-0.713100

H	0.000000	12.001164	-1.246583
C	0.000000	11.054548	0.713100
H	0.000000	12.001164	1.246583
C	0.000000	9.872578	1.407452
H	0.000000	9.870003	2.494972
H	0.000000	9.870003	-2.494972

[6]-CC: CS-B3LYP geometry

C	1.209261	2.094520	1.401665
C	2.420053	0.000000	1.401617
C	1.209261	-2.094520	1.401665
C	-1.209261	-2.094520	1.401665
C	-2.420053	0.000000	1.401617
C	-1.209261	2.094520	1.401665
H	1.193833	-2.067962	2.489381
H	2.389591	0.000000	2.489316
H	1.193833	2.067962	2.489381
H	-1.193833	2.067962	2.489381
H	-1.193833	-2.067962	2.489381
H	-2.389591	0.000000	2.489316
C	-2.076106	1.198537	0.725811
C	0.000000	2.398270	0.725726
C	2.076106	1.198537	0.725811
C	2.076106	-1.198537	0.725811
C	0.000000	-2.398270	0.725726
C	-2.076106	-1.198537	0.725811
C	0.000000	2.398270	-0.725726
C	2.076106	1.198537	-0.725811
C	-2.076106	1.198537	-0.725811
C	0.000000	-2.398270	-0.725726
C	-2.076106	-1.198537	-0.725811
C	2.076106	-1.198537	-0.725811
H	1.193833	2.067962	-2.489381
H	1.193833	-2.067962	-2.489381
H	-2.389591	0.000000	-2.489316
H	-1.193833	2.067962	-2.489381
H	2.389591	0.000000	-2.489316
H	-1.193833	-2.067962	-2.489381
C	1.209261	2.094520	-1.401665
C	2.420053	0.000000	-1.401617
C	1.209261	-2.094520	-1.401665
C	-1.209261	-2.094520	-1.401665
C	-2.420053	0.000000	-1.401617
C	-1.209261	2.094520	-1.401665

[6]-CC: BS-UB3LYP geometry

C	1.209552	2.094944	1.405402
C	2.420720	0.000000	1.405383
C	1.209552	-2.094944	1.405402
C	-1.209552	-2.094944	1.405402
C	-2.420720	0.000000	1.405383
C	-1.209552	2.094944	1.405402
H	1.190539	-2.062128	2.492709
H	2.383078	0.000000	2.492675
H	1.190539	2.062128	2.492709
H	-1.190539	2.062128	2.492709
H	-1.190539	-2.062128	2.492709
H	-2.383078	0.000000	2.492675
C	-2.079879	1.200687	0.725754
C	0.000000	2.402481	0.725677
C	2.079879	1.200687	0.725754
C	2.079879	-1.200687	0.725754
C	0.000000	-2.402481	0.725677
C	-2.079879	-1.200687	0.725754
C	0.000000	2.402481	-0.725677
C	2.079879	1.200687	-0.725754
C	-2.079879	1.200687	-0.725754
C	0.000000	-2.402481	-0.725677
C	-2.079879	-1.200687	-0.725754
C	2.079879	-1.200687	-0.725754
H	1.190539	2.062128	-2.492709
H	1.190539	-2.062128	-2.492709
H	-2.383078	0.000000	-2.492675
H	-1.190539	2.062128	-2.492709
H	2.383078	0.000000	-2.492675
H	-1.190539	-2.062128	-2.492709
C	1.209552	2.094944	-1.405402
C	2.420720	0.000000	-1.405383
C	1.209552	-2.094944	-1.405402
C	-1.209552	-2.094944	-1.405402
C	-2.420720	0.000000	-1.405383
C	-1.209552	2.094944	-1.405402

[8]-CC: CS-B3LYP geometry

C	-1.217587	2.939516	1.406307
C	-2.939516	1.217587	1.406307
C	-2.939516	-1.217587	1.406307
C	-1.217587	-2.939516	1.406307
C	1.217587	-2.939516	1.406307

C	2.939516	-1.217587	1.406307
C	2.939516	1.217587	1.406307
C	1.217587	2.939516	1.406307
H	2.914510	-1.207230	2.494030
H	1.207230	-2.914510	2.494030
H	-1.207230	-2.914510	2.494030
H	-2.914510	-1.207230	2.494030
H	-2.914510	1.207230	2.494030
H	-1.207230	2.914510	2.494030
H	1.207230	2.914510	2.494030
H	2.914510	1.207230	2.494030
C	0.000000	3.165955	0.729611
C	-2.238668	2.238668	0.729611
C	-3.165955	0.000000	0.729611
C	-2.238668	-2.238668	0.729611
C	0.000000	-3.165955	0.729611
C	2.238668	-2.238668	0.729611
C	3.165955	0.000000	0.729611
C	2.238668	2.238668	0.729611
C	-2.238668	2.238668	-0.729611
C	0.000000	3.165955	-0.729611
C	-3.165955	0.000000	-0.729611
C	2.238668	2.238668	-0.729611
C	3.165955	0.000000	-0.729611
C	2.238668	-2.238668	-0.729611
C	0.000000	-3.165955	-0.729611
C	-2.238668	-2.238668	-0.729611
H	2.914510	-1.207230	-2.494030
H	1.207230	-2.914510	-2.494030
H	-1.207230	-2.914510	-2.494030
H	-2.914510	-1.207230	-2.494030
H	-2.914510	1.207230	-2.494030
H	-1.207230	2.914510	-2.494030
H	1.207230	2.914510	-2.494030
H	2.914510	1.207230	-2.494030
C	-1.217587	2.939516	-1.406307
C	-2.939516	1.217587	-1.406307
C	-2.939516	-1.217587	-1.406307
C	-1.217587	-2.939516	-1.406307
C	1.217587	-2.939516	-1.406307
C	1.217587	2.939516	-1.406307
C	2.939516	-1.217587	-1.406307
C	2.939516	1.217587	-1.406307

[8]-CC: BS-UB3LYP geometry

C	2.813541	1.489001	1.408487
C	0.936536	3.042448	1.408467
C	-1.489007	2.813556	1.408450
C	-3.042454	0.936552	1.408444
C	-2.813562	-1.488991	1.408455
C	-0.936558	-3.042438	1.408474
C	1.488985	-2.813547	1.408492
C	3.042433	-0.936542	1.408497
H	-0.927146	-3.012441	2.496010
H	-2.786125	-1.474453	2.495980
H	-3.012469	0.927136	2.495980
H	-1.474480	2.786115	2.495975
H	0.927108	3.012458	2.496003
H	2.786087	1.474470	2.496012
H	3.012431	-0.927119	2.496033
H	1.474442	-2.786097	2.496017
C	3.155879	0.297753	0.729025
C	2.020809	2.441755	0.729034
C	-0.297756	3.155887	0.728988
C	-2.441758	2.020817	0.729001
C	-3.155890	-0.297748	0.728978
C	-2.020820	-2.441750	0.729020
C	0.297745	-3.155882	0.729015
C	2.441747	-2.020812	0.729053
C	2.020820	2.441750	-0.729020
C	3.155890	0.297748	-0.728978
C	-0.297745	3.155882	-0.729015
C	2.441758	-2.020817	-0.729001
C	0.297756	-3.155887	-0.728988
C	-2.020809	-2.441755	-0.729034
C	-3.155879	-0.297753	-0.729025
C	-2.441747	2.020812	-0.729053
H	-0.927108	-3.012458	-2.496003
H	-2.786087	-1.474470	-2.496012
H	-3.012431	0.927119	-2.496033
H	-1.474442	2.786097	-2.496017
H	0.927146	3.012441	-2.496010
H	2.786125	1.474453	-2.495980
H	3.012469	-0.927136	-2.495980
H	1.474480	-2.786115	-2.495975
C	2.813562	1.488991	-1.408455
C	0.936558	3.042438	-1.408474
C	-1.488985	2.813547	-1.408492
C	-3.042433	0.936542	-1.408497
C	-2.813541	-1.489001	-1.408487
C	3.042454	-0.936552	-1.408444
C	-0.936536	-3.042448	-1.408467

C   1.489007   -2.813556   -1.408450

[10]-CC: CS-B3LYP geometry

```
  C    -1.221591     3.759672     1.408255
C     1.221591     3.759672     1.408255
C     3.198168     2.323605     1.408255
C     3.953153     0.000000     1.408255
C     3.198168    -2.323605     1.408255
C     1.221591    -3.759672     1.408255
C    -1.221591    -3.759672     1.408255
C    -3.198168    -2.323605     1.408255
C    -3.953153     0.000000     1.408255
C    -3.198168     2.323605     1.408255
H     3.929807     0.000000     2.496071
H     3.179280    -2.309882     2.496071
H     1.214377    -3.737468     2.496071
H     1.214377     3.737468     2.496071
H    -1.214377     3.737468     2.496071
H    -3.179280     2.309882     2.496071
H    -3.929807     0.000000     2.496071
H    -3.179280    -2.309882     2.496071
H    -1.214377    -3.737468     2.496071
H     3.179280     2.309882     2.496071
C     0.000000     3.940483     0.731560
C     2.316158     3.187918     0.731560
C     3.747622     1.217676     0.731560
C     3.747622    -1.217676     0.731560
C     2.316158    -3.187918     0.731560
C     0.000000    -3.940483     0.731560
C    -2.316158    -3.187918     0.731560
C    -3.747622    -1.217676     0.731560
C    -3.747622     1.217676     0.731560
C    -2.316158     3.187918     0.731560
C     0.000000     3.940483    -0.731560
C     2.316158     3.187918    -0.731560
C     3.747622    -1.217676    -0.731560
C     2.316158    -3.187918    -0.731560
C     0.000000    -3.940483    -0.731560
C    -2.316158    -3.187918    -0.731560
C    -3.747622    -1.217676    -0.731560
C    -3.747622     1.217676    -0.731560
C    -2.316158     3.187918    -0.731560
C     3.747622     1.217676    -0.731560
H     1.214377    -3.737468    -2.496071
```

H	3.179280	-2.309882	-2.496071
H	3.929807	0.000000	-2.496071
H	3.179280	2.309882	-2.496071
H	1.214377	3.737468	-2.496071
H	-1.214377	3.737468	-2.496071
H	-3.179280	2.309882	-2.496071
H	-3.929807	0.000000	-2.496071
H	-3.179280	-2.309882	-2.496071
H	-1.214377	-3.737468	-2.496071
C	1.221591	3.759672	-1.408255
C	-1.221591	3.759672	-1.408255
C	-3.198168	2.323605	-1.408255
C	-3.953153	0.000000	-1.408255
C	-3.198168	-2.323605	-1.408255
C	-1.221591	-3.759672	-1.408255
C	1.221591	-3.759672	-1.408255
C	3.198168	-2.323605	-1.408255
C	3.953153	0.000000	-1.408255
C	3.198168	2.323605	-1.408255

[10]-CC: BS-UB3LYP geometry

C	-1.223125	3.764391	1.409384
C	1.223125	3.764391	1.409384
C	3.202182	2.326522	1.409384
C	3.958115	0.000000	1.409384
C	3.202182	-2.326522	1.409384
C	1.223125	-3.764391	1.409384
C	-1.223125	-3.764391	1.409384
C	-3.202182	-2.326522	1.409384
C	-3.958115	0.000000	1.409384
C	-3.202182	2.326522	1.409384
H	3.929875	0.000000	2.497162
H	3.179336	-2.309923	2.497162
H	1.214398	-3.737533	2.497162
H	1.214398	3.737533	2.497162
H	-1.214398	3.737533	2.497162
H	-3.179336	2.309923	2.497162
H	-3.929875	0.000000	2.497162
H	-3.179336	-2.309923	2.497162
H	-1.214398	-3.737533	2.497162
H	3.179336	2.309923	2.497162
C	0.000000	3.947327	0.730175
C	2.320180	3.193454	0.730175
C	3.754131	1.219791	0.730175
C	3.754131	-1.219791	0.730175

```
C      2.320180    -3.193454     0.730175
C      0.000000    -3.947327     0.730175
C     -2.320180    -3.193454     0.730175
C     -3.754131    -1.219791     0.730175
C     -3.754131     1.219791     0.730175
C     -2.320180     3.193454     0.730175
C      0.000000     3.947327    -0.730175
C      2.320180     3.193454    -0.730175
C      3.754131    -1.219791    -0.730175
C      2.320180    -3.193454    -0.730175
C      0.000000    -3.947327    -0.730175
C     -2.320180    -3.193454    -0.730175
C     -3.754131    -1.219791    -0.730175
C     -3.754131     1.219791    -0.730175
C     -2.320180     3.193454    -0.730175
C      3.754131     1.219791    -0.730175
H      1.214398    -3.737533    -2.497162
H      3.179336    -2.309923    -2.497162
H      3.929875     0.000000    -2.497162
H      3.179336     2.309923    -2.497162
H      1.214398     3.737533    -2.497162
H     -1.214398     3.737533    -2.497162
H     -3.179336     2.309923    -2.497162
H     -3.929875     0.000000    -2.497162
H     -3.179336    -2.309923    -2.497162
H     -1.214398    -3.737533    -2.497162
C      1.223125     3.764391    -1.409384
C     -1.223125     3.764391    -1.409384
C     -3.202182     2.326522    -1.409384
C     -3.958115     0.000000    -1.409384
C     -3.202182    -2.326522    -1.409384
C     -1.223125    -3.764391    -1.409384
C      1.223125    -3.764391    -1.409384
C      3.202182    -2.326522    -1.409384
C      3.958115     0.000000    -1.409384
C      3.202182     2.326522    -1.409384
```

[12]-CC: CS-B3LYP geometry

```
C     -2.918352    -3.721341     1.409514
C     -0.666614    -4.681303     1.409509
C      1.763514    -4.387544     1.409457
C      3.721340    -2.918352     1.409514
C      4.681302    -0.666614     1.409509
C      4.387543     1.763515     1.409457
```

C	2.918352	3.721341	1.409514
C	0.666614	4.681304	1.409509
C	-1.763514	4.387544	1.409457
C	-3.721340	2.918353	1.409514
C	-4.681302	0.666614	1.409509
C	-4.387543	-1.763514	1.409457
H	-4.368110	-1.755576	2.497237
H	-4.368110	-1.755576	-2.497237
H	-4.660051	0.663522	-2.497277
H	-4.660051	0.663522	2.497277
H	-3.704755	2.905423	2.497307
H	-3.704755	2.905423	-2.497307
H	-1.755576	4.368111	-2.497237
H	-1.755576	4.368111	2.497237
H	0.663522	4.660053	2.497277
H	0.663522	4.660053	-2.497277
H	2.905423	3.704756	-2.497307
H	2.905423	3.704756	2.497307
C	-3.773571	-2.833017	0.732611
C	-1.851656	-4.340217	0.732659
C	0.566525	-4.684099	0.732609
C	2.833016	-3.773572	0.732611
C	4.340216	-1.851657	0.732659
C	4.684097	0.566525	0.732609
C	3.773571	2.833016	0.732611
C	1.851656	4.340217	0.732659
C	-0.566526	4.684098	0.732609
C	-2.833016	3.773571	0.732611
C	-4.340216	1.851656	0.732659
C	-4.684097	-0.566526	0.732609
C	-3.773571	-2.833017	-0.732611
C	-1.851656	-4.340217	-0.732659
C	0.566525	-4.684099	-0.732609
C	2.833016	-3.773572	-0.732611
C	4.340216	-1.851657	-0.732659
C	4.684097	0.566525	-0.732609
C	3.773571	2.833016	-0.732611
C	1.851656	4.340217	-0.732659
C	-0.566526	4.684098	-0.732609
C	-4.340216	1.851656	-0.732659
C	-4.684097	-0.566526	-0.732609
C	-2.918352	-3.721341	-1.409514
H	4.368110	1.755576	2.497237
H	4.368110	1.755576	-2.497237
H	4.660051	-0.663522	-2.497277
H	4.660051	-0.663522	2.497277
H	3.704754	-2.905423	2.497307

H	3.704754	-2.905423	-2.497307
H	1.755575	-4.368111	-2.497237
H	1.755575	-4.368111	2.497237
H	-0.663522	-4.660052	2.497277
H	-0.663522	-4.660052	-2.497277
H	-2.905422	-3.704755	-2.497307
H	-2.905422	-3.704755	2.497307
C	-0.666614	-4.681303	-1.409509
C	1.763514	-4.387544	-1.409457
C	3.721340	-2.918352	-1.409514
C	4.681302	-0.666614	-1.409509
C	4.387543	1.763515	-1.409457
C	2.918352	3.721341	-1.409514
C	0.666614	4.681304	-1.409509
C	-1.763514	4.387544	-1.409457
C	-3.721340	2.918353	-1.409514
C	-4.681302	0.666614	-1.409509
C	-4.387543	-1.763514	-1.409457
C	-2.833016	3.773571	-0.732611

[12]-CC: BS-UB3LYP geometry

C	-3.801498	2.825403	1.409411
C	-4.704085	0.545966	1.409433
C	-4.347228	-1.879485	1.409363
C	-2.825403	-3.801498	1.409411
C	-0.545966	-4.704086	1.409433
C	1.879485	-4.347229	1.409363
C	3.801498	-2.825403	1.409411
C	4.704085	-0.545966	1.409433
C	4.347228	1.879485	1.409363
C	2.825403	3.801498	1.409411
C	0.545966	4.704086	1.409433
C	-1.879485	4.347228	1.409363
H	-1.870797	4.327188	2.497210
H	-1.870797	4.327188	-2.497210
H	0.543352	4.681853	-2.497274
H	0.543352	4.681853	2.497274
H	2.812114	3.783539	2.497243
H	2.812114	3.783539	-2.497243
H	4.327187	1.870796	-2.497210
H	4.327187	1.870796	2.497210
H	4.681852	-0.543352	2.497274
H	4.681852	-0.543352	-2.497274
H	3.783538	-2.812114	-2.497243

H	3.783538	-2.812114	2.497243
C	-2.934853	3.705458	0.730236
C	-4.394232	1.741682	0.730271
C	-4.675575	-0.688783	0.730195
C	-3.705457	-2.934853	0.730236
C	-1.741683	-4.394233	0.730271
C	0.688783	-4.675576	0.730195
C	2.934853	-3.705458	0.730236
C	4.394232	-1.741682	0.730271
C	4.675575	0.688783	0.730195
C	3.705457	2.934853	0.730236
C	1.741682	4.394233	0.730271
C	-0.688783	4.675576	0.730195
C	-2.934853	3.705458	-0.730236
C	-4.394232	1.741682	-0.730271
C	-4.675575	-0.688783	-0.730195
C	-3.705457	-2.934853	-0.730236
C	-1.741683	-4.394233	-0.730271
C	0.688783	-4.675576	-0.730195
C	2.934853	-3.705458	-0.730236
C	4.394232	-1.741682	-0.730271
C	4.675575	0.688783	-0.730195
C	1.741682	4.394233	-0.730271
C	-0.688783	4.675576	-0.730195
C	-3.801498	2.825403	-1.409411
H	1.870797	-4.327188	2.497210
H	1.870797	-4.327188	-2.497210
H	-0.543353	-4.681853	-2.497274
H	-0.543353	-4.681853	2.497274
H	-2.812114	-3.783538	2.497243
H	-2.812114	-3.783538	-2.497243
H	-4.327187	-1.870796	-2.497210
H	-4.327187	-1.870796	2.497210
H	-4.681852	0.543352	2.497274
H	-4.681852	0.543352	-2.497274
H	-3.783538	2.812114	-2.497243
H	-3.783538	2.812114	2.497243
C	-4.704085	0.545966	-1.409433
C	-4.347228	-1.879485	-1.409363
C	-2.825403	-3.801498	-1.409411
C	-0.545966	-4.704086	-1.409433
C	1.879485	-4.347229	-1.409363
C	3.801498	-2.825403	-1.409411
C	4.704085	-0.545966	-1.409433
C	4.347228	1.879485	-1.409363
C	2.825403	3.801498	-1.409411
C	0.545966	4.704086	-1.409433

| C | -1.879485 | 4.347228 | -1.409363 |
| C | 3.705457 | 2.934853 | -0.730236 |

[7]-CC: CS-B3LYP geometry

C	-1.209240	2.511012	1.416254
C	1.209240	2.511012	1.416254
C	2.717137	0.620169	1.416254
C	2.178975	-1.737674	1.416254
C	0.000000	-2.787013	1.416254
C	-2.178975	-1.737674	1.416254
C	-2.717137	0.620169	1.416254
H	-1.188326	2.467584	2.502733
H	1.188326	2.467584	2.502733
H	2.670144	0.609443	2.502733
H	2.141289	-1.707621	2.502733
H	0.000000	-2.738812	2.502733
H	-2.670144	0.609443	2.502733
H	-2.141289	-1.707621	2.502733
C	0.000000	2.778829	0.735536
C	2.172576	1.732572	0.735536
C	2.709158	-0.618348	0.735536
C	1.205689	-2.503639	0.735536
C	-2.172576	1.732572	0.735536
C	-1.205689	-2.503639	0.735536
C	-2.709158	-0.618348	0.735536
C	-2.172576	1.732572	-0.735536
C	-2.709158	-0.618348	-0.735536
C	-1.205689	-2.503639	-0.735536
C	1.205689	-2.503639	-0.735536
C	2.709158	-0.618348	-0.735536
C	2.172576	1.732572	-0.735536
C	0.000000	2.778829	-0.735536
H	-2.670144	0.609443	-2.502733
H	-2.141289	-1.707621	-2.502733
H	0.000000	-2.738812	-2.502733
H	2.141289	-1.707621	-2.502733
H	2.670144	0.609443	-2.502733
H	1.188326	2.467584	-2.502733
H	-1.188326	2.467584	-2.502733
C	1.209240	2.511012	-1.416254
C	-1.209240	2.511012	-1.416254
C	2.717137	0.620169	-1.416254
C	2.178975	-1.737674	-1.416254
C	0.000000	-2.787013	-1.416254
C	-2.178975	-1.737674	-1.416254

C	-2.717137	0.620169	-1.416254

[7]-CC: BS-UB3LYP geometry

C	-1.215008	1.410028	-2.523473
C	1.215008	1.410028	-2.523473
C	2.729773	1.410072	-0.623081
C	2.189356	1.410068	1.746349
C	0.000000	1.409970	2.800731
C	-2.189356	1.410068	1.746349
C	-2.729773	1.410072	-0.623081
H	-1.198102	2.497351	-2.488212
H	1.198102	2.497351	-2.488212
H	2.691890	2.497424	-0.614210
H	2.158488	2.497394	1.721968
H	0.000000	2.497242	2.760595
H	-2.691890	2.497424	-0.614210
H	-2.158488	2.497394	1.721968
C	0.000000	0.728855	-2.787838
C	2.178649	0.728879	-1.737782
C	2.716891	0.728919	0.620178
C	1.209349	0.728836	2.511389
C	-2.178649	0.728879	-1.737782
C	-1.209349	0.728836	2.511389
C	-2.716891	0.728919	0.620178
C	-2.178649	-0.728879	-1.737782
C	-2.716891	-0.728919	0.620178
C	-1.209349	-0.728836	2.511389
C	1.209349	-0.728836	2.511389
C	2.716891	-0.728919	0.620178
C	2.178649	-0.728879	-1.737782
C	0.000000	-0.728855	-2.787838
H	-2.691890	-2.497424	-0.614210
H	-2.158488	-2.497394	1.721968
H	0.000000	-2.497242	2.760595
H	2.158488	-2.497394	1.721968
H	2.691890	-2.497424	-0.614210
H	1.198102	-2.497351	-2.488212
H	-1.198102	-2.497351	-2.488212
C	1.215008	-1.410028	-2.523473
C	-1.215008	-1.410028	-2.523473
C	2.729773	-1.410072	-0.623081
C	2.189356	-1.410068	1.746349
C	0.000000	-1.409970	2.800731
C	-2.189356	-1.410068	1.746349
C	-2.729773	-1.410072	-0.623081

[9]-CC: CS-B3LYP geometry

C	3.082242	1.415510	-1.779707
C	3.504874	1.415489	0.618031
C	2.287824	1.415560	2.726705
C	0.000000	1.415609	3.559799
C	-2.287824	1.415560	2.726705
C	-3.504874	1.415489	0.618031
C	-3.082242	1.415510	-1.779707
C	-1.217382	1.415538	-3.345138
C	1.217382	1.415538	-3.345138
H	-3.047903	2.502340	-1.759909
H	-3.466083	2.502345	0.611262
H	-2.262551	2.502424	2.696638
H	0.000000	2.502436	3.520245
H	2.262551	2.502424	2.696638
H	3.466083	2.502345	0.611262
H	3.047903	2.502340	-1.759909
H	1.203936	2.502406	-3.308620
H	-1.203936	2.502406	-3.308620
C	0.000000	0.734815	-3.552829
C	2.283519	0.734847	-2.721590
C	3.498377	0.734830	-0.616888
C	1.215042	0.734844	3.338909
C	3.076141	0.734804	1.776277
C	-1.215042	0.734844	3.338909
C	-3.076141	0.734804	1.776277
C	-3.498377	0.734830	-0.616888
C	-2.283519	0.734847	-2.721590
C	0.000000	-0.734815	-3.552829
C	2.283519	-0.734847	-2.721590
C	3.498377	-0.734830	-0.616888
C	3.076141	-0.734804	1.776277
C	1.215042	-0.734844	3.338909
C	-1.215042	-0.734844	3.338909
C	-3.076141	-0.734804	1.776277
C	-3.498377	-0.734830	-0.616888
C	-2.283519	-0.734847	-2.721590
H	-3.047903	-2.502340	-1.759909
H	-3.466083	-2.502345	0.611262
H	-2.262551	-2.502424	2.696638
H	1.203936	-2.502406	-3.308620
H	3.047903	-2.502340	-1.759909

H	3.466083	-2.502345	0.611262
H	2.262551	-2.502424	2.696638
H	0.000000	-2.502436	3.520245
H	-1.203936	-2.502406	-3.308620
C	1.217382	-1.415538	-3.345138
C	3.082242	-1.415510	-1.779707
C	3.504874	-1.415489	0.618031
C	2.287824	-1.415560	2.726705
C	-2.287824	-1.415560	2.726705
C	-3.504874	-1.415489	0.618031
C	-3.082242	-1.415510	-1.779707
C	-1.217382	-1.415538	-3.345138
C	0.000000	-1.415609	3.559799

[9]-CC: BS-UB3LYP geometry

C	3.095168	1.408715	-1.787072
C	3.519570	1.408694	0.620619
C	2.297355	1.408755	2.738005
C	0.000000	1.408815	3.574520
C	-2.297355	1.408755	2.738005
C	-3.519570	1.408694	0.620619
C	-3.095168	1.408715	-1.787072
C	-1.222441	1.408710	-3.358900
C	1.222441	1.408710	-3.358900
H	-3.069455	2.496380	-1.772284
H	-3.490647	2.496382	0.615542
H	-2.278552	2.496456	2.715523
H	0.000000	2.496478	3.544836
H	2.278552	2.496456	2.715523
H	3.490647	2.496382	0.615542
H	3.069455	2.496380	-1.772284
H	1.212291	2.496410	-3.331598
H	-1.212291	2.496410	-3.331598
C	0.000000	0.728211	-3.562188
C	2.289625	0.728257	-2.728791
C	3.507827	0.728229	-0.618564
C	1.218273	0.728288	3.347671
C	3.084377	0.728212	1.780933
C	-1.218273	0.728288	3.347671
C	-3.084377	0.728212	1.780933
C	-3.507827	0.728229	-0.618564
C	-2.289625	0.728257	-2.728791
C	0.000000	-0.728211	-3.562188
C	2.289625	-0.728257	-2.728791
C	3.507827	-0.728229	-0.618564

```
C     3.084377     -0.728212      1.780933
C     1.218273     -0.728288      3.347671
C    -1.218273     -0.728288      3.347671
C    -3.084377     -0.728212      1.780933
C    -3.507827     -0.728229     -0.618564
C    -2.289625     -0.728257     -2.728791
H    -3.069455     -2.496380     -1.772284
H    -3.490647     -2.496382      0.615542
H    -2.278552     -2.496456      2.715523
H     1.212291     -2.496410     -3.331598
H     3.069455     -2.496380     -1.772284
H     3.490647     -2.496382      0.615542
H     2.278552     -2.496456      2.715523
H     0.000000     -2.496478      3.544836
H    -1.212291     -2.496410     -3.331598
C     1.222441     -1.408710     -3.358900
C     3.095168     -1.408715     -1.787072
C     3.519570     -1.408694      0.620619
C     2.297355     -1.408755      2.738005
C    -2.297355     -1.408755      2.738005
C    -3.519570     -1.408694      0.620619
C    -3.095168     -1.408715     -1.787072
C    -1.222441     -1.408710     -3.358900
C     0.000000     -1.408815      3.574520
```

[11]-CC: CS-B3LYP geometry

```
C     3.646198     -2.344261      1.414989
C     4.333772      0.000000      1.414979
C     3.646198      2.344261      1.414989
C     1.800964      3.945392      1.414936
C    -0.617066      4.293459      1.415005
C    -2.838712      3.277333      1.415032
C    -4.158397      1.221509      1.414985
C    -4.158397     -1.221509      1.414985
C    -2.838712     -3.277333      1.415032
C    -0.617066     -4.293459      1.415005
C     1.800964     -3.945392      1.414936
H     1.787221     -3.915710     -2.502055
H     1.787221     -3.915710      2.502055
H    -0.612251     -4.260660     -2.502109
H    -0.612251     -4.260660      2.502109
H    -2.817060     -3.252468     -2.502148
H    -2.817060     -3.252468      2.502148
H    -4.127144     -1.212374     -2.502106
H    -4.127144     -1.212374      2.502106
```

H	-4.127144	1.212374	-2.502106
H	-4.127144	1.212374	2.502106
H	-2.817060	3.252468	-2.502148
C	4.152652	-1.219851	0.734565
C	4.152652	1.219851	0.734565
C	2.834992	3.273129	0.734576
C	0.616203	4.287743	0.734546
C	-1.798623	3.940281	0.734616
C	-3.641047	2.340989	0.734557
C	-4.328078	0.000000	0.734613
C	-3.641047	-2.340989	0.734557
C	-1.798623	-3.940281	0.734616
C	0.616203	-4.287743	0.734546
C	2.834992	-3.273128	0.734576
C	4.152652	-1.219851	-0.734565
C	4.152652	1.219851	-0.734565
C	2.834992	3.273129	-0.734576
C	0.616203	4.287743	-0.734546
C	-1.798623	3.940281	-0.734616
C	-3.641047	2.340989	-0.734557
C	-4.328078	0.000000	-0.734613
C	-3.641047	-2.340989	-0.734557
C	-1.798623	-3.940281	-0.734616
C	0.616203	-4.287743	-0.734546
C	2.834992	-3.273128	-0.734576
H	-2.817060	3.252468	2.502148
H	-0.612251	4.260660	-2.502109
H	-0.612251	4.260660	2.502109
H	1.787221	3.915710	-2.502055
H	1.787221	3.915710	2.502055
H	3.618456	2.326537	-2.502102
H	3.618456	2.326537	2.502102
H	4.301444	0.000000	2.502107
H	4.301444	0.000000	-2.502107
H	3.618456	-2.326537	-2.502102
H	3.618456	-2.326537	2.502102
C	3.646198	2.344261	-1.414989
C	1.800964	3.945392	-1.414936
C	-0.617066	4.293459	-1.415005
C	-2.838712	3.277333	-1.415032
C	-4.158397	1.221509	-1.414985
C	-4.158397	-1.221509	-1.414985
C	-2.838712	-3.277333	-1.415032
C	-0.617066	-4.293459	-1.415005
C	1.800964	-3.945392	-1.414936
C	3.646198	-2.344261	-1.414989
C	4.333772	0.000000	-1.414979

[11]-CC: BS-UB3LYP geometry

C	3.658733	-2.352228	1.408428
C	4.348677	0.000000	1.408420
C	3.658733	2.352228	1.408428
C	1.807138	3.958747	1.408362
C	-0.619146	4.307964	1.408432
C	-2.848424	3.288442	1.408452
C	-4.172721	1.225671	1.408408
C	-4.172721	-1.225672	1.408408
C	-2.848424	-3.288442	1.408452
C	-0.619146	-4.307964	1.408432
C	1.807138	-3.958747	1.408362
H	1.797222	-3.937513	-2.496210
H	1.797222	-3.937513	2.496210
H	-0.615648	-4.284398	-2.496270
H	-0.615648	-4.284398	2.496270
H	-2.832981	-3.270648	-2.496301
H	-2.832981	-3.270648	2.496301
H	-4.150445	-1.219155	-2.496257
H	-4.150445	-1.219155	2.496257
H	-4.150445	1.219155	-2.496257
H	-4.150445	1.219155	2.496257
H	-2.832981	3.270648	-2.496301
C	4.162176	-1.222618	0.728745
C	4.162176	1.222618	0.728745
C	2.841478	3.280531	0.728765
C	0.617598	4.297386	0.728717
C	-1.802718	3.949124	0.728799
C	-3.649383	2.346258	0.728722
C	-4.338098	0.000000	0.728774
C	-3.649383	-2.346258	0.728722
C	-1.802718	-3.949124	0.728799
C	0.617598	-4.297386	0.728717
C	2.841478	-3.280531	0.728765
C	4.162176	-1.222618	-0.728745
C	4.162176	1.222618	-0.728745
C	2.841478	3.280531	-0.728765
C	0.617598	4.297386	-0.728717
C	-1.802718	3.949124	-0.728799
C	-3.649383	2.346258	-0.728722
C	-4.338098	0.000000	-0.728774
C	-3.649383	-2.346258	-0.728722
C	-1.802718	-3.949124	-0.728799
C	0.617598	-4.297386	-0.728717

C	2.841478	-3.280531	-0.728765
H	-2.832981	3.270648	2.496301
H	-0.615648	4.284398	-2.496270
H	-0.615648	4.284398	2.496270
H	1.797222	3.937513	-2.496210
H	1.797222	3.937513	2.496210
H	3.638889	2.339567	-2.496271
H	3.638889	2.339567	2.496271
H	4.325678	0.000000	2.496269
H	4.325678	0.000000	-2.496269
H	3.638889	-2.339567	-2.496271
H	3.638889	-2.339567	2.496271
C	3.658733	2.352228	-1.408428
C	1.807138	3.958747	-1.408362
C	-0.619146	4.307964	-1.408432
C	-2.848424	3.288442	-1.408452
C	-4.172721	1.225671	-1.408408
C	-4.172721	-1.225672	-1.408408
C	-2.848424	-3.288442	-1.408452
C	-0.619146	-4.307964	-1.408432
C	1.807138	-3.958747	-1.408362
C	3.658733	-2.352228	-1.408428
C	4.348677	0.000000	-1.408420